CompassCDS
User Guide

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Contents

Introduction 3
Software Presentation 3
Getting Started 4
Connection 4
Starting an Acquisition 4
How to View an Acquisition 8
Reprocessing a Chromatogram 11
Starting a Sequence 14
Application Details 16
Software Structure 16
The Method 38
CompassCDS Variables 110
Baseline Monitoring / Quick Start / Sequence 139
The Calibration Curves 160
Manual Integration and Identification 170
Reprocessing a Chromatogram 173
Viewing the Results 180
Integration Results Display on the Chromatogram 180
Summary Report 194
Importing a Chromatogram (AIA format) 204
Audit Trail 204
How to Compare Two Chromatograms 207
Electronic Signature 208
Lock/Unlock Chromatograms 222
Advanced Parameters 225
IntelliUpdate 225
Remote Sequence 227
Retention Index 232
CompassCDS ASCII Import 240
CompassCDS Print manager (PDF Export) 240
CompassCDS Arithmetic functions 240
Procedures 241
How to Acquire a Chromatogram 241
How to Define a Sequence for Analysis Execution 244
How to Build a Process Method 245
How to Reprocess a Chromatogram 247
How to Build a Calibration Curve 249
How to Print a Customized Report 250
How to Print a Calibration Curve 252
Glossary 253

Introduction

Software Presentation

CompassCDS is a state-of-the-art, chromatography software platform that provides a choice of complete pull-down task menus, user-friendly icons, and easily accessible popup menus within specific windows. The browser and task wizards enable new users to quickly complete their tasks, making CompassCDS a very “easy to learn” chromatography software.

CompassCDS can acquire data from GC systems. The control methods for such instruments are fully integrated within the CompassCDS interface.

CompassCDS is able to effectively integrate most chromatograms automatically using only two parameters: peak width and noise threshold which are entered at time zero. These parameters are automatically updated and the system applies the optimum values for each chromatogram. In some cases specific integration events may be required to integrate complex chromatograms. These are readily available within CompassCDS. Reference peaks may also be used for peak identification, and several calibration modes are available including normalization, external or internal standard, with response factors or calibration curves. CompassCDS can also quantify peaks within a group using a common response factor or calibration curve.

CompassCDS enables users to define custom variables via a unique variable editor and to also summarize reports with control charts and tables which can be built to monitor the evolution of analysis results. System suitability tests can also be performed automatically on all CompassCDS variables, including user-defined custom variables.

Customized analysis reports can be configured within CompassCDS Report Editor, the CompassCDS custom report editor. Chromatograms, results tables, calibration reports, etc. with customized formatting and presentation can be inserted and then saved as a report style file. Report styles can be recalled later or edited and saved as another report style file.

The use of the individual instrument control drivers, CompassCDS Configuration Manager, CompassCDS Report Editor, the report builder, and all optional processing modules are explained in detail in separate user guides that are provided with the corresponding applications.

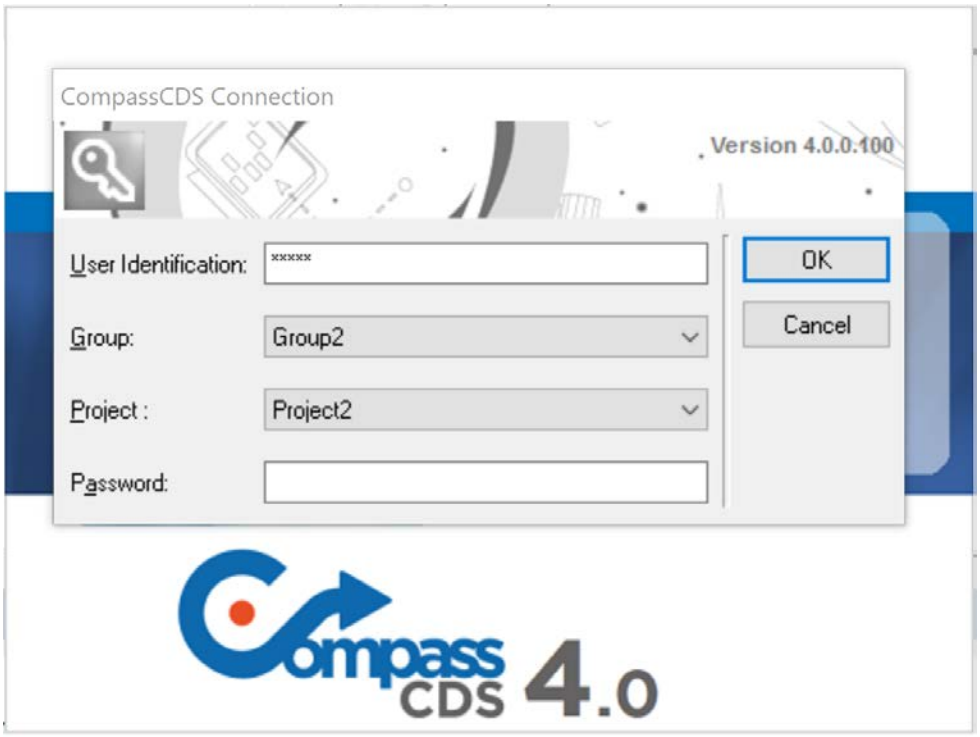
How to use this manual when using CompassCDS for the first time

Start by reading the "Getting Started" section. This section contains essential information about acquisition and chromatogram handling. More detailed information for each individual function can be found in the section “Application details.”

Getting Started

Connection

If the default domain is defined during the installation, the following logon box is displayed when starting CompassCDS:



The user must enter their ‘User identification’, and choose in the scroll box the group and the project in which to work and, if necessary, type in a password. The password is case sensitive, meaning that abc is different from ABC. User names and passwords will be assigned by the system administrator or can be set by logging into the CompassCDS Configuration Manager application, using an administrator login, and creating/editing a user.

When a user connects for the first time, the user will be asked to change the password.

Starting an Acquisition

The first step is the creation of a method, which then enables the acquisition of chromatograms. This method will be associated with the chromatogram once the data has been acquired.

Creating the Method

From the menu, select FILE / NEW / NEW METHOD.

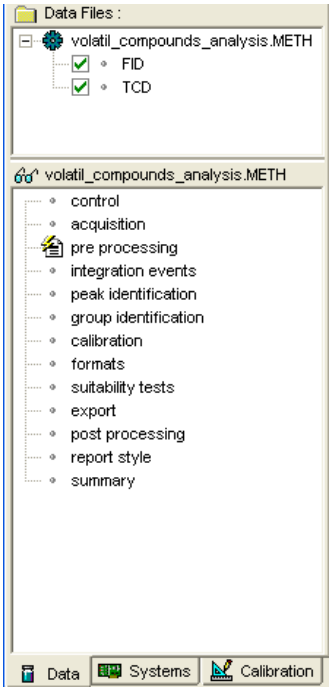
Select the project in which the method will be used (when in all projects mode) and the chromatographic system, to which the method will be applied.

Click Next.

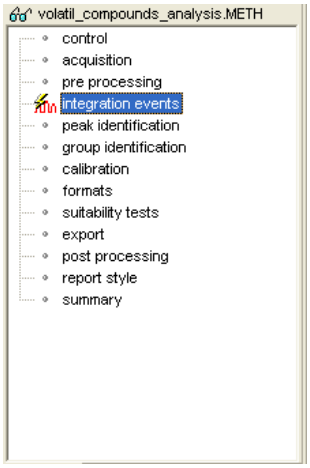
Enter the name of the method, and a method description (optional) which will appear as a comment in the Open File window. The un-edited method is opened with default settings and parameters listed in each section of the method tree.

To display the different sections of a method (acquisition parameters, integration parameters, etc.), click on the corresponding item in the method tree. Methods created for multi-channel instruments will show both channels in the top section of the browser as shown below. To select a channel, a user clicks on that channel and the method tree corresponding to that channel will appear in the browser.

To select the FID channel …



To select a method section in the method tree…



Defining Method Parameters

In the method tree in the browser, clicking on the control section displays the parts of a method associated with instrument control.

If the instrument is being fully controlled by CompassCDS, a user can enter the required instrument control method parameters.

In the method tree in the browser, clicking on the acquisition section displays the fields associated with each injection such as Run Name, Run Time, Injection volume.

Parameters set in this section will appear by default in the acquisition start windows (Quick Start and sequence). For example, the run name can be entered (the identifier or suffix will be implemented automatically for each run in the case of a Quick Start) and the run length.

NOTE: In the chromatograms acquired, the parameters of this field will be the ones entered for the acquisition. If a reprocess of the acquired chromatogram is done, the acquisition parameters will not change in this field.

In the method tree in the browser, clicking on the Integration section displays the fields associated with integrating chromatograms.

This section enables a user to set the integration parameters required for the correct integration of chromatograms. In the case of simple chromatograms, the two default parameter settings should be sufficient to integrate the chromatogram. Entering the approximate width of the peak of interest in the peak width parameter box, and a value for the 'threshold' to define the start and the end of a peak, according to the slope of the signal and then re-integrating (F5) enables users to optimize the integration parameter settings for specific analyses

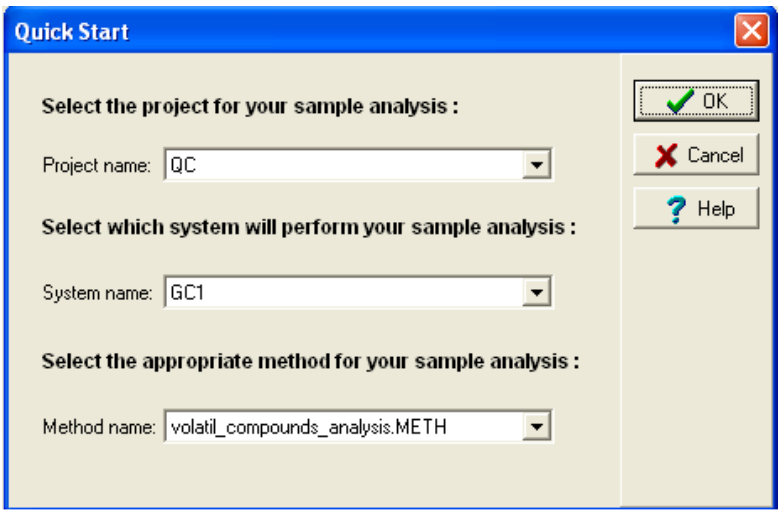
These parameters are all that are required to start an acquisition. Other method parameters, e.g., “Peak Identification”, “Calibration” or “Grouping”, can be selected later once example data for the application exists.

Save the method by using the pull-down menu selection

FILE / SAVE / SAVE METHOD, clicking on the Save Method icon or by pressing the key combination Shift+Ctrl+2.

Starting an Acquisition

Selecting ACQUISITION / QUICK START from the pull-down menu brings up the Quick Start window.


Quick Start
Select the project for your sample analysis :
Project name: QC
Select which system will perform your sample analysis :
System name: GC1
Select the appropriate method for your sample analysis :
Method name: volatil_compounds_analysis.METH
OK
Cancel
Help

The three fields in this window are filled in by either typing names or selecting these from the drop-down lists:

- The project (if connecting into CompassCDS in all projects). If the all projects option is not selected for a user (default state) then only the following two fields are displayed.
- The chromatographic system or instrument on which sample is to be analyzed.
- The name of the analysis method.

Clicking on OK displays a window for entering or confirming the acquisition parameters.

The following minimum set of parameters must be entered:

- The chromatogram name (File Name and Run identifier that will be used to create the name).
- The acquisition run time in minutes.

If a CompassCDS controlled system is configured with a fully controlled autosampler the following additional information must be entered:

- The injection volume.
- The vial number in the tray and, if necessary, the rack number.

Pressing Start once the acquisition parameters have been entered will start an acquisition.

If the system is not using an autosampler, the sample can be manually injected and pressing start on the chromatograph will initiate acquisition.

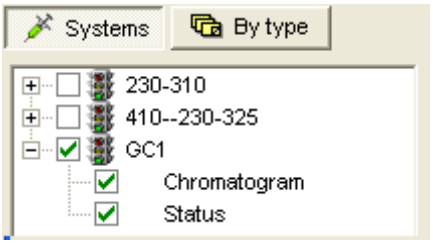
How to View an Acquisition

Viewing an Acquisition

From the CompassCDS main screen, click on the Systems tab (bottom left of window) to go to the Systems view.

In the browser, a user then selects the system into which the sample was injected by checking the appropriate checkbox. Clicking the chromatogram checkbox enables users to view the data acquisition. Clicking the status checkbox enables users to also view the system status.

NOTE: The ✔ symbol in front of the system name indicates that the system is selected. By default, both 'chromatogram' and 'status' are selected when the system checkbox is selected.



An idle system is preceded by the symbol, while a system which is busy downloading a method or waiting for an injection in preceded by , and a running system is preceded by .

The chromatogram(s) is displayed and refreshed automatically throughout the entire acquisition.

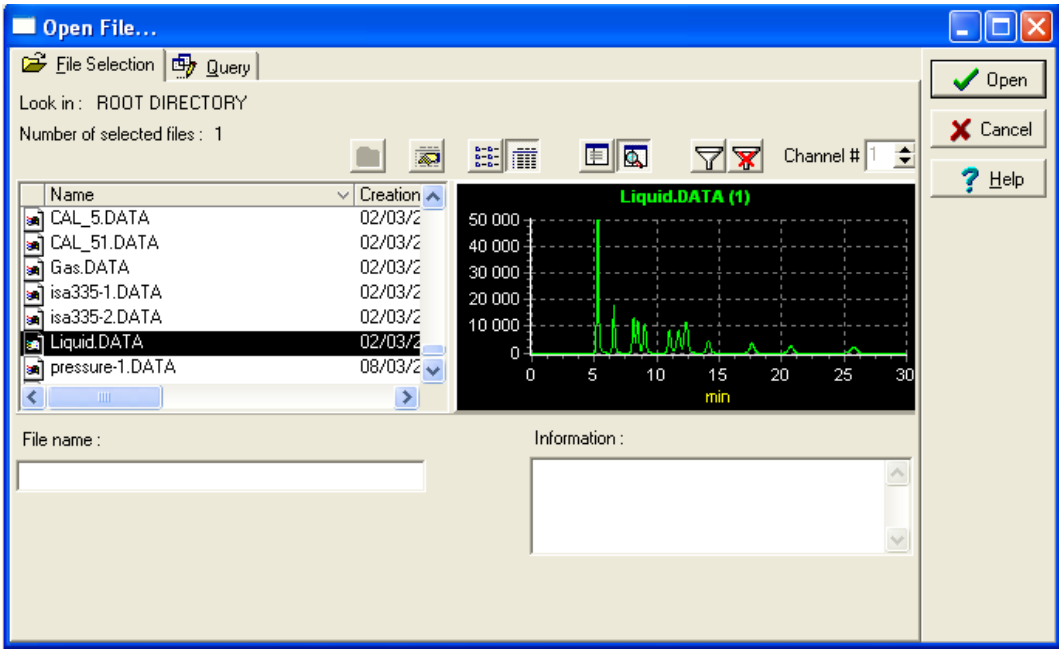
In order to stop an acquisition before the end of a run, a user can press the *Stop* button . If the chromatographic system is not fully controlled (e.g.,, data acquisition only), the data acquisition process will be terminated. If the system is fully controlled, the button will stop either only acquisition or acquisition and the chromatographic system according to the driver configuration.

In this case, the chromatograph remains active, e.g., in the case of a GC, although data acquisition has stopped, the oven temperature program will continue and the chromatograph may have to be stopped manually.

Viewing a Chromatogram

Once the chromatogram has been acquired, it can be opened and processed:

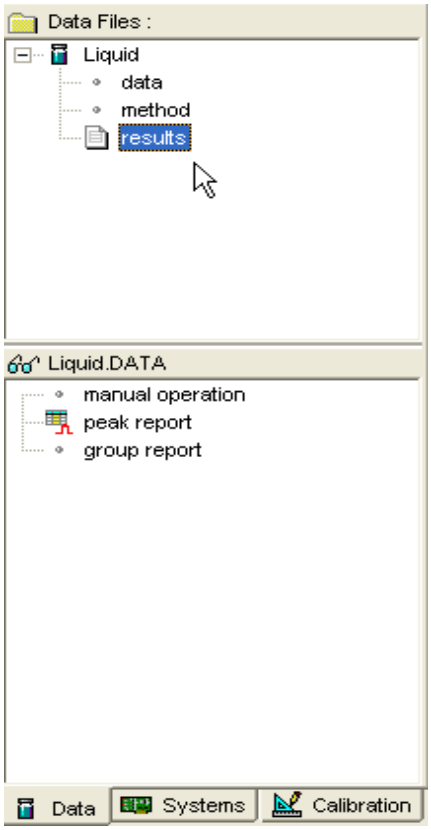
Selecting FILE / OPEN / OPEN CHROMATOGRAM or pressing causes the Open File window to appear:



In this window, users can use the scroll bars to scroll down the list and click on the most recently acquired chromatogram. Alternatively, typing the first few letters of the chromatogram name in the file name box will display only the chromatograms with names beginning with these letters. Clicking on the Open button or double clicking on the selected chromatogram will cause it to be displayed in the Data view.

The selected chromatogram, which will have already been processed and the results table, will be displayed on the screen.

In the browser, click on Results to view the integration results table.

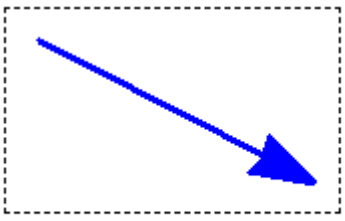


Clicking on Peak report enables users to view the results calculations for each peak.

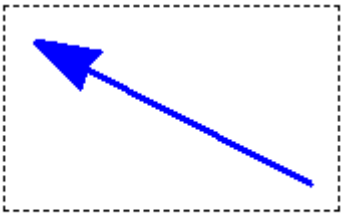
The peak report is displayed in the right panel below the chromatogram.

The results (peak names, baseline, and integration marker) are also displayed on the chromatogram.

Users can zoom in or out of a displayed chromatogram by clicking and dragging the left mouse button. Top left to the bottom right of the screen will zoom in and bottom left to top right will un-zoom.

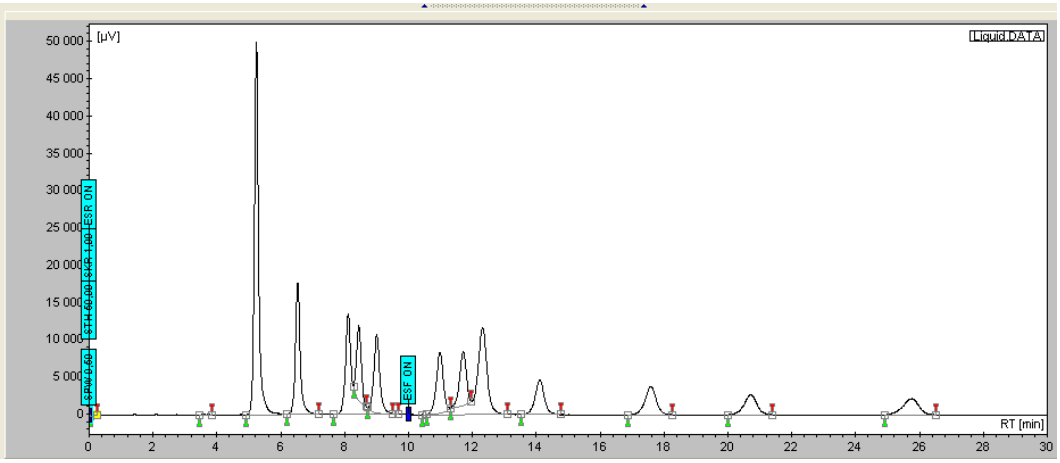


Zoom in



Zoom out

Clicking on the bar directly a displayed chromatogram will display or hide the chromatogram.



Reprocessing a Chromatogram

Once the chromatogram is opened, it is possible to modify the chromatogram results. This may be done either by modifying the method associated with the chromatogram or by modifying the integration or the identification manually.

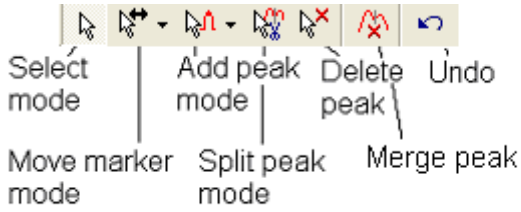
Integration

In automatic mode:

Change the integration events in the corresponding section of the method, and press F5 or click on the *Calculate* icon to view the changes.

In manual mode:

Use the manual integration bar to manually modify the integration.



In Select mode, click on a marker to select the corresponding peak, then select the icon corresponding to the desired action.

In Move marker mode, click on the marker to move, and then click on the new marker location.

In Add peak mode, click where the peak should start, then click where the peak should stop.

In Split peak mode, click on the place the peak should be split.

In Delete peak mode, the currently selected peak is deleted. THEREFORE, MAKE THE PEAK SELECTION BEFORE CLICKING ON THE DELETE PEAK ICON. (The selected peak markers and report line are highlighted in yellow).

In Merge peak mode, the currently selected peak is deleted and the next peak is extended to the left in order to include the deleted peak. This option is available only if peaks are separated by a valley or have been split.

Each time the integration events are modified manually, the modification action is saved within the Manual operation and can be removed using the Undo icon . Click on Results/Manual integration in the browser to view the manual modifications.

Identification

In automatic mode:

Change the identification table and press F5 or the Integrate icon to view the changes.

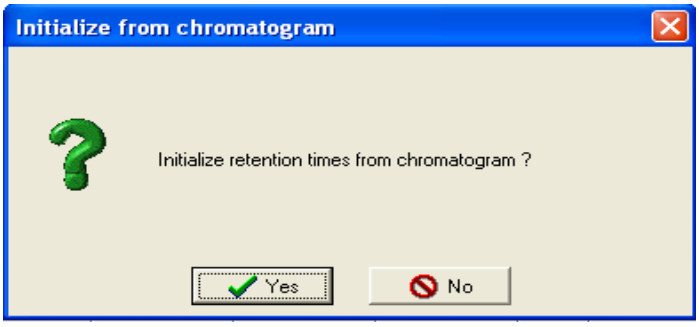
In manual mode:

Display the result table (click on Results/Peak report in the browser), then edit the peak names in the table. Double-click in the 'Name' column and type the new name to rename the peak manually.

As with manual integration, this operation is saved in the Manual events and can be removed with the Undo icon .

If the identification is not correct, it is possible to rename the peaks manually and then update the changes in the identification method:

Select Method and then Identification in the browser. To update the retention windows, press the right mouse button in the identification table and select Initialize retention times from chromatogram. Answer yes to the confirmation message:



Reprocessing

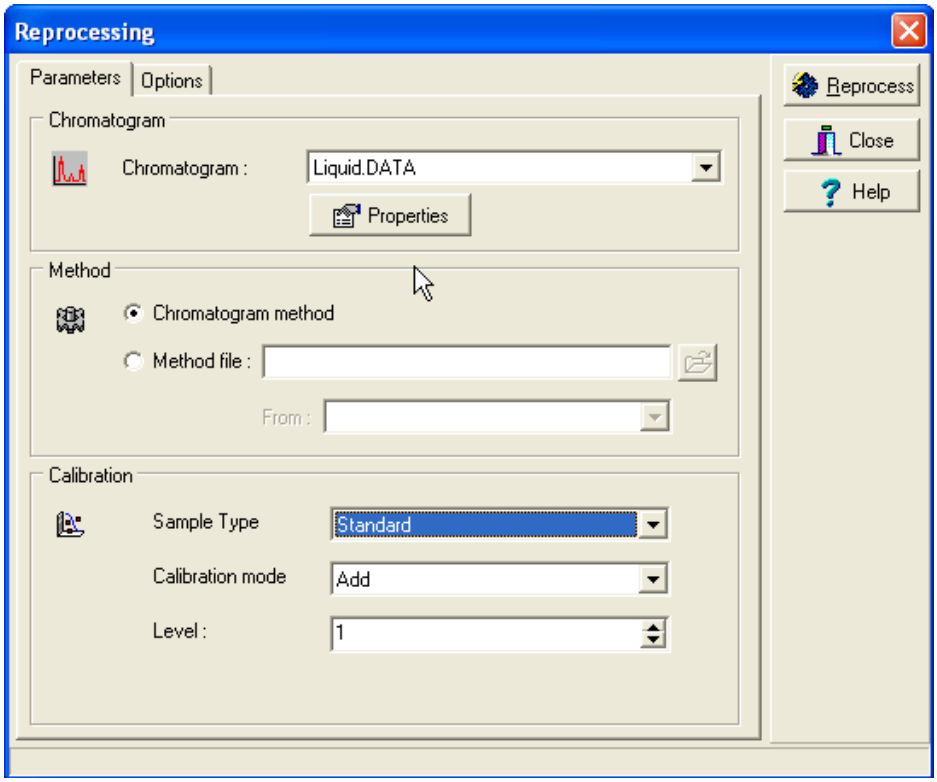
If the Identification section, Integration section, or the Variables are changed, press *F5* or click on the *Integrate* icon to view the changes.

If the Export, Post Processing, Print report or Summary sections are changed, the chromatogram must be reprocessed.

If the Calibration section is changed, recalculating is sufficient only if the analysis performed is for an Unknown sample. However, if the sample is a Standard, then this sample must be reprocessed by clicking on the r*eprocess* icon or by pressing the F6 key.

To reprocess a chromatogram, select PROCESSING / REPROCESS.

The Reprocessing window appears:



In this window, select the name of the chromatogram to process from the list of all the open chromatogram names. The selected chromatogram is chosen by default.

Now select the method to be used to process the chromatogram. By default, the chromatogram will be processed with the method associated with it. If the chromatogram must be reprocessed with an external method, check the Method file option, and press to select the method name in the Open File window.

In the Calibration area, select Unknown if the chromatogram is an unknown sample or Standard Level X if the sample is a standard corresponding to the Level X in the Calibration method. In the case of a standard (the calibration section of the method has to be correctly completed first), check “Clear old points” to delete previous calibration points or check “Clear this level only” to delete the points corresponding to the same standard level. Do not check anything to add a point to an existing calibration curve.

By accessing the Option pages, it is possible to uncheck some of the processing features so that they will not be run during the processing. In the case of a two-channel method, the "Options" page is divided into 2 tabs (one for each channel). Thus, it is possible to perform some actions on one channel and others on the second one.

Once all the parameters are set, press the Reprocess button to start the reprocessing. A message in the status bar at the bottom of the screen indicates that the calculation is completed.

NOTE: If the chromatogram has been treated as a standard, a calibration curve is generated. To display this curve, select the menu FILE / OPEN / OPEN CALIBRATION CURVE, and select the name of the calibration curve. The corresponding curve(s) is/are displayed on the right page.

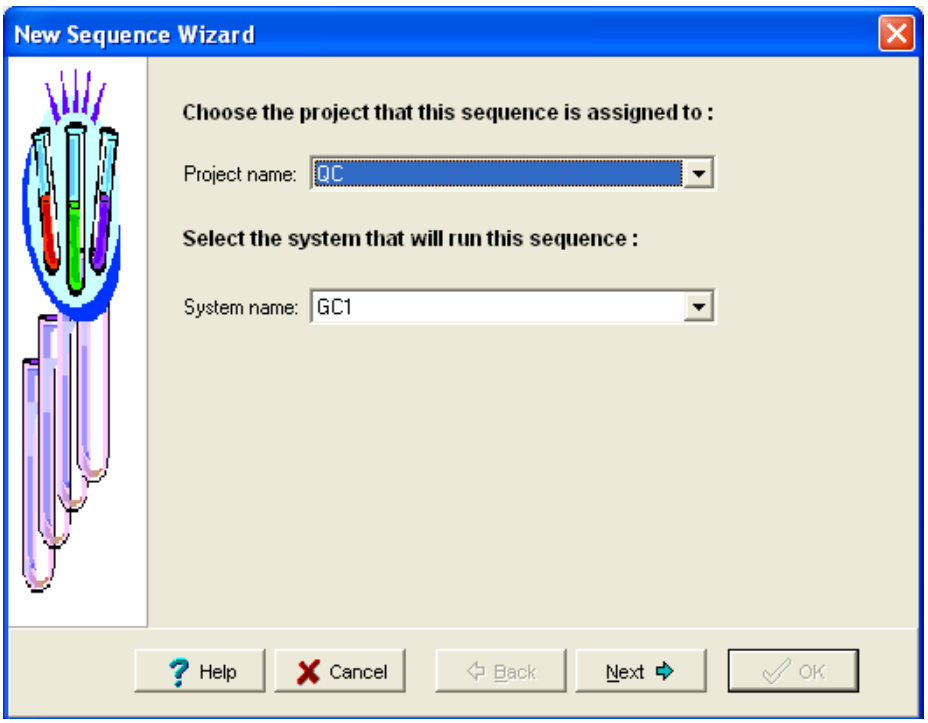
NOTE: If the properties of the chromatogram are modified, they will not be displayed in its acquisition part (which cannot be overwritten), but the new values will be visible in the variable part as global variables.

Starting a Sequence

To start several acquisitions at the same time, the corresponding processing methods need to be first created. It is then possible to create the sequence.

In the main menu, select FILE / NEW / NEW SEQUENCE:

A window appears for selecting which system is to be used to inject the samples:



Select the project (if connected in all projects) and the system and press Next, enter the number of lines (samples) for the sequence and press OK.

NOTE: Only one system can be used by sequence.

In the Browser, a new object is added corresponding to this sequence.

Click on the Icon '+' to add additional sample lines to the sequence table.

In each line of the sequence, enter the name of the method that will be used for acquisition, processing, and editing of the chromatogram.

Some cells of the line are filled automatically with the parameters entered in the acquisition part of the method.

The minimum parameters that must be entered are:

- The chromatogram name (File prefix and Run identifier that will be used to create the name).
- The acquisitions run time in minutes.
- The user input variables if some have been defined in the method with a mandatory feature.
- The istd values, if an internal standard calibration has been defined in the method.

If CompassCDS controls an autosampler:

- The injection volume.
- The vial number in the tray and, if necessary, the rack number.

To fill the cells quickly, use the ‘Fill block’ icon . (Or the fill block option in the popup menu), for example, fill-in the first RunID (suffix) cell, then select this cell with all the cells to be filled, and press the ‘Fill block’ icon .

A window called ‘Auto fill block’ appears.

Press OK.

The cells are filled with incremented integers or a copy of the first cell.

Save the sequence, and then launch the sequence with the Run icon .

Application Details

Software Structure

Logon

When initially starting the CompassCDS, a logon is required that will identify each person with a user name and the project(s) and group in which the work will be performed. This amounts to specifying a working directory, a profile, etc. The working directory is the directory where the data are stored, i.e., the file path when opening or saving a file. The profile is defined for a user or several users and specifies the rights to perform the various actions in CompassCDS. If a menu or a certain button is deactivated, the user does not have the access privilege or rights to perform the corresponding action. A prompt for password entry may also be required for certain tasks.

Users with the right to log on all projects will have the possibility to choose “All projects” as the project name. This enables them to view all files in all projects and to control all instruments assigned to the projects. This special privilege is defined in the user properties in CompassCDS Configuration Manager.

The user, group, and project names are defined in CompassCDS Configuration Manager.

The name, group, and project for the user are displayed in the CompassCDS status bar, at the bottom of the main screen.

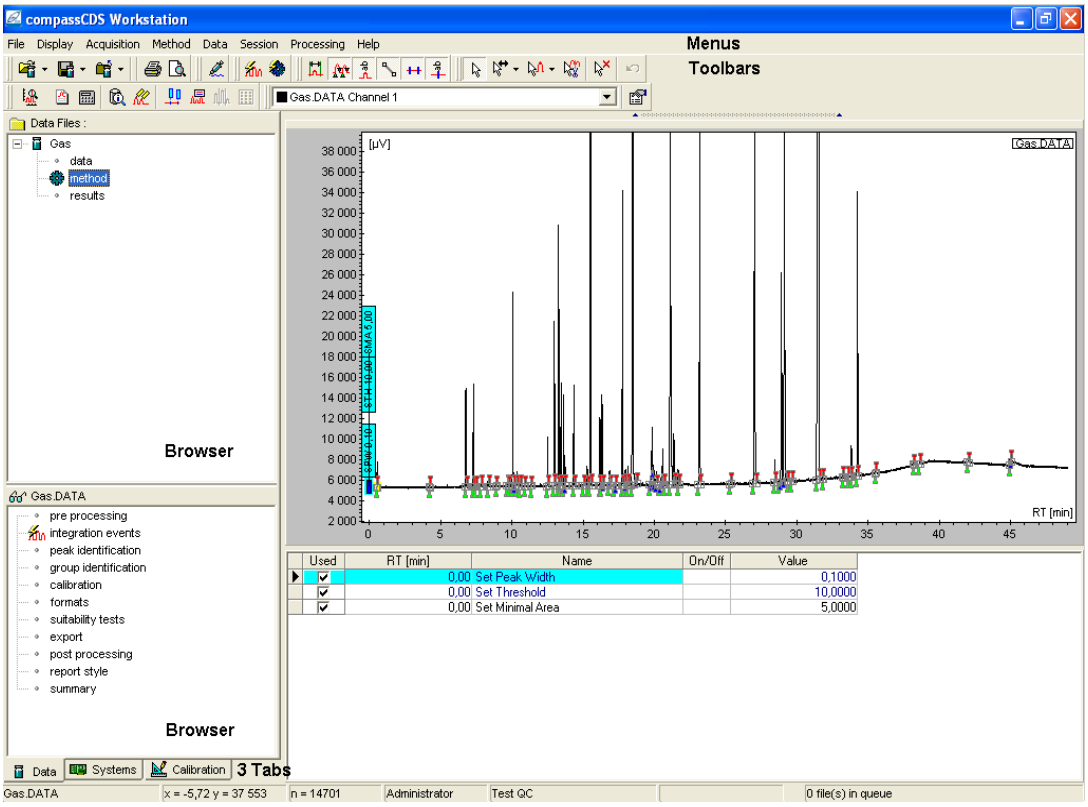
In order to change the name of the user connected or to change the group, it is necessary to logon again: Select SESSION / NEW LOGIN from the menu and a new connection window will appear as for the first logon session to CompassCDS as described above.

Any user with administrator rights can change passwords in the CompassCDS Configuration Manager. However, a user can change his password in the CompassCDS using the menu SESSION / CHANGE PASSWORD, if the user has been assigned the right to modify the password (this option is defined in the user properties in the CompassCDS Configuration Manager).

Screen Construction

The CompassCDS screen consists of a main menu, toolbars for specific tasks, a browser, three tabs, and a status bar.

The main menu provides access to most of the software functions. However, more specific tasks can be performed using the toolbars. The popup menus also provide access to many functions. Click the right mouse button within the window of interest to make the popup menu appear. All tables and graphics use popup menus.



The bar displayed above the chromatogram

May be used to hide the chromatogram, and when selected in the browser, this can be useful to display in full page the content of a selected part of the chromatogram's method. This bar is only active in post run data files.

Main Menu

Available Menus:

File menu- manages the files and configures the software and the printing.

Display menu- displays or hides toolbars; the audit trails and configures chromatogram view parameters.

Acquisition menu- starts a single acquisition, a baseline monitoring or a Remote Sequence (see page 139).

Method menu- configures the method.

Data menu- manages opened chromatograms: selection of chromatograms and viewing of chromatogram properties.

Session menu- displays information about the connected user and enables a change in logon.

Processing menu- recalculates or reprocesses the results of a chromatogram.

Help menu- provides quick access to information about software features.

The Toolbars

The toolbars provide rapid access to most CompassCDS functions. These toolbars can be displayed or hidden.

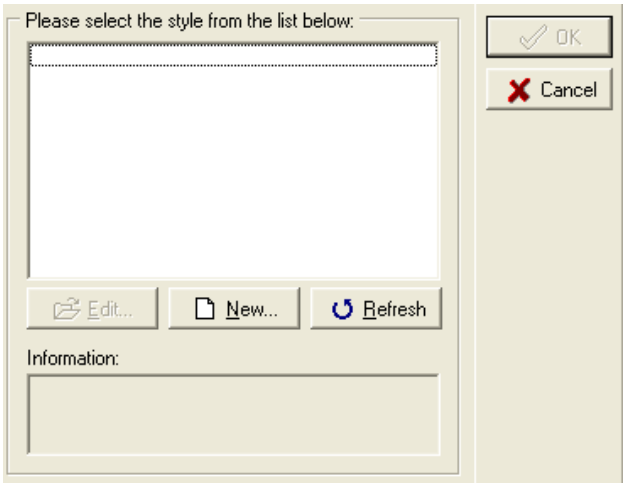
Select the menu option DISPLAY / TOOLBARS, and a window appears with a list of all toolbars that can be hidden or shown. Simply check the box next to the named toolbar in order to display it, each unchecked box indicates that the toolbar will not be displayed.

File Bar

This toolbar provides access to the file management features: open, save, close, printing, lock and Esign. These functions are available for chromatogram, method, sequence, reprocessing list.

Once a chromatogram is selected or has been opened, the first three icons can open, save, or close chromatograms. In the same way, when opening or selecting a method, a sequence a calibration curve, a reprocessing list etc. the three icons will manage the corresponding file, and their properties are modified accordingly. For example: to open a method and to open a sequence.

: To generate a PDF file on the template of the CompassCDS Report Editor report style defined in the “Report style” part of the method. The file has the name of the chromatogram plus the creation date and time with a PDF extension. If the chromatogram is signed electronically, “signed” is mentioned in the PDF file name (after the name and the date and time). To open the PDF generated file, use Acrobat reader (free on the web site www.acrobat.com) and included on the CompassCDS CD-ROM, or any PDF compatible reader utility : If a chromatogram is selected, the associated report (report style part of the method) is printed. If a method or a calibration curve is selected, the following screen is displayed:



The User selects a defined report in the list. The user can edit it by pressing the Edit button, create a new one by pressing the NEW button, or refresh the list by pressing the Refresh button.

: To have a preview of the report before its printing.

: These features are displayed only if corresponding profile is associated to the connected user. Use them to lock or unlock chromatograms files.

Electronic Signature Bar

This toolbar displayed only if the corresponding profile is associated to the connected user, provides access to (in order):

: The chromatogram signature option.

: The signature of a batch of chromatograms option.

: The list of signatures made on a chromatogram.

Display Bar

This toolbar provides access to (in order):

: to display the identification window of identified peaks centered on the experimental retention time, (if the user has defined reference peaks, and that a peak which has a theoretical retention time defined in the identification table of 3 minutes and has an actual retention time of 4.2 minutes, the window displayed is centered around 4.2 minutes). The user has to place the mouse cursor onto the name of a peak in the peak identification table to display its identification window.

: To display the start and end markers of integrated peaks.

: To display annotations of peaks (it can be the name of the peak, its retention time, etc., according to what is selected in the chromatogram annotation bar, or in the format/chromatogram section of a method).

: To display the baseline.

: To display the integration event markers.

: To display the integration event annotation selected in the chromatogram annotation bar, or in the format/chromatogram section of a method.

Chromatogram Annotation Bar

Use this toolbar to select the way to display the chromatogram on the screen.

This toolbar provides access to (in order):

: To display the Workspace, used to define the type of chromatogram view (overlay, stack, full screen), and the scale.

: To display the properties of a peak: distribution of acquired points, inflection points, etc.

: To display the audit trail of the selected object.

: To configure the way to annotate peaks.

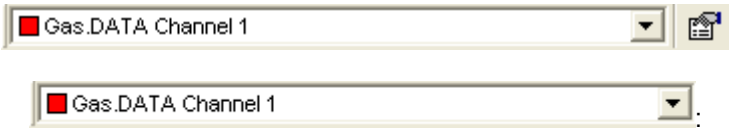
: To configure the way to annotate integration events.

: To configure annotations and markers displayed on the chromatogram.

Acquisition Bar

Starts Quick Start

Data Bar



Chromatogram name: allows the selecting and displaying of an opened chromatogram.

: Chromatogram properties: to display the properties of a chromatogram: variables, information, sample properties, etc.

Processing Bar

: To reintegrate a chromatogram after changes: In the integration part, calibration (if it is an unknown only), peak and group identification.

: To reprocess a chromatogram, this function allows you to perform all the functions, accessible from the method.

Manual Integration Bar

(refer to page 170)

This toolbar provides access to (in order):

	To select the peak for which the integration has to be modified.
	To move the peak markers.
	To add a new peak by defining its start and end.
	To split a peak into two peaks.
	To remove a peak
	To merge two peaks
	To delete the last manual operation performed.

Every manual change executed is listed in the part results/manual operations of the chromatogram.

NOTE: To unlock a toolbar and make it a separate moveable window, click at the left side of a toolbar then drag it to the desired location.

The Browser

The browser is displayed at the left part of the application window to permit viewing of opened files names.

The browser can be hidden. If it is not visible, select the menu option DISPLAY and check BROWSER.

At the bottom of the browser are three tabs: Data, Systems, and Calibration. Click on Data to view the chromatograms, sequences, methods and the reprocessing list that are opened. Click on Systems to display the running acquisitions. Click on Calibration to edit the calibration curves.

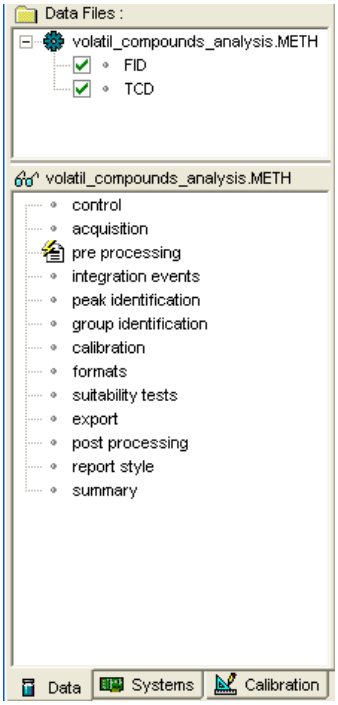
Press the right mouse button on any item displayed in the browser to view a popup menu to provide faster access to options when performing certain tasks.

To Display a Method

Select the menu option FILE / OPEN / OPEN METHOD and double-click on the file name to be opened.

The name of the method is displayed in the browser. The method can be a multi-channel method. In this case, the sub-methods for each channel are shown above the name of the method. By clicking on one or another channel, the right panel display will be updated corresponding to the selected channel.

The method is composed of several sections (Control, Acquisition, Integration, etc.). Each section can be displayed in the right panel by clicking in the bottom part of the browser.



The name of the method, under which the channel sub-methods are listed, is also displayed in the space between the two parts of the browser.

Click the right mouse button on the method to view its popup menu. The popup menu of a method is:

CLOSE METHOD	To close the method
SAVE METHOD	To save the method
SAVE METHOD AS	To save a method under a new name.
SAVE METHOD AS TEMPLATE	To save the method as a template.
PRINT	To print the method report.
AUDIT TRAIL	To display the audit trail of the method.

The popup menu of the grids (displayed in the right part of the screen) contains a Copy option that allows the grid content to be copied for pasting into another application (Word, Excel).

To view a Chromatogram

Select the menu option FILE / OPEN / OPEN CHROMATOGRAM and double-click on the file name to open.

The name of the chromatogram is displayed in the browser. A chromatogram is saved with the method used to process it and the results.

- Click on Data to view the chromatogram in the right panel.
- Click on Method to display the method. The method is composed of several sections (Control, Acquisition, Integration, etc.). These sub-methods are displayed in the right panel by clicking on them in the bottom part of the browser.

NOTE: To hide the chromatogram when displayed above the method, uncheck the menu option DISPLAY / DATA VISIBLE, or click on the bar above it:

- Click on Results to view the calculation results in the right panel. The results include the manual operations, peak table, and group table. Click on each element to obtain the corresponding results on the right panel

Press the right mouse button on the chromatogram name displayed in the browser to view its popup menu. The following options are available.

CLOSE CHROMATOGRAM	To close the chromatogram without using the Close chromatogram window.
SAVE CHROMATOGRAM	To save the chromatogram.
SAVE METHOD AS TEMPLATE	To save the method of the chromatogram as template.
PRINT	To print the chromatogram report.
DATA VISIBLE	Check or uncheck this menu to show or hide the chromatogram in the right panel, when method or results parts are selected.
AUDIT TRAIL	To view the processing history of the chromatogram, a list of the operations made with the chromatogram is given.
CHROMATOGRAM PROPERTIES	View the chromatogram properties ( ), and parameters such as the sample mass, the internal standard mass and all the global variables, including the user input variables.

Press the right mouse button on the data part of the chromatogram in the browser, the DATA VISIBLE option is available in the popup menu.

Press the right mouse button on the method name of the chromatogram in the browser to view its popup menu. The following options are available.

UPDATE METHOD	To update the last method used to reprocess the chromatogram with the chromatogram processing parameters
SAVE METHOD AS	To save the method as a new method, with a new name.
SAVE METHOD AS TEMPLATE	To save the method of the chromatogram as template
AUDIT TRAIL	To view the processing history of the chromatogram. A list of the operations made with the chromatogram is given.

To view a Sequence

Select the menu option FILE / OPEN / OPEN SEQUENCE and double-click on the file name to open.

The name of the sequence is displayed in the browser. Click on it to display the sequence in the right part of the application.

Press the right mouse button on the sequence displayed in the browser to view its popup menu. The popup menu of a sequence is:

CLOSE SEQUENCE	To close the sequence: it is not possible to close a running sequence.
SAVE SEQUENCE	To save the sequence.
SAVE SEQUENCE AS	To save the sequence under a new name, so that the original sequence file is not lost (overwritten).
PRINT	To print the sequence.

To view a Reprocessing List

Select the menu option FILE / OPEN / OPEN REPROCESSING LIST and double-click on the file name to open it.

The name of the reprocessing list is displayed in the browser. Click on it to display the reprocessing list in the right part of the application.

Click the right mouse button on a reprocessing list displayed in the browser to view its popup menu. The popup menu of a reprocessing list is:

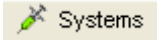
CLOSE REPROCESSING LIST	To close the reprocessing list.
SAVE REPROCESSING LIST	To save the reprocessing list.
SAVE REPROCESSING LIST AS	To save the reprocessing list under a new name, so that the original reprocessing list is not lost (overwritten).
PRINT	To print the reprocessing list.

To View an Acquisition

Click on the System tab set at the bottom of the browser. The list of all accessible chromatographs (dependent upon user access rights and group/project definition) is displayed in the browser.

For each chromatograph (or system), the active chromatogram, as well as system status (particularly interesting if the system has a fully controlled autosampler) and general information about the run can be viewed during the live acquisition.

This information can be displayed “by system” or “by type”:

Press the 

button to view all information concerning one system in the same window. When this button is pressed, choose which information will be displayed for each system by checking the corresponding objects.

Press the By type button to view only one type of information (acquisition or status), for a few or all of these systems (check the corresponding systems).

A maximum of 2 chromatograms or 2 status displays can be viewed by page.

Click on the right mouse button on an item displayed in the browser to view its popup menu.

To view a Calibration Curve

Click on the Calibration tab at the bottom of the browser.

Select the menu option FILE / OPEN / OPEN CALIBRATION CURVE and double-click on the file name in order to open the selected file.

A calibration curve consists of several curves, one for each compound calibrated in the chromatogram. In the browser, click on the compound to display the corresponding curve in the right panel

All previous versions of a calibration curve are not completely deleted, but archives can be created if the user allows it, (defined in CompassCDS Configuration Manager). The archives can be sorted by date or by name:

- Press the Arch / button to sort them by compound.
- Press the Arch / button to sort them by date.
- Press the Cur. button to view the current curves.

NOTE: The archiving date of a file corresponds to the date at which the calibration curve has been replaced, i.e., the creation date of the new curve. The calibration curve creation date appears in the right screen.

The Status Bar

The status bar at the bottom of the main screen displays information about the software status:

File name zone: Displays the name of the selected file (and channel in the case of multi-channel chromatograms and methods).

Process zone: Displays a progress bar during a calculation or any other task indicating that the system is busy. When the system is available, by pointing the cursor inside a curve, the coordinates of the cursor position are also displayed in this zone.

Point's number (n=): If a chromatogram is selected, this field indicates the number of points constituting this chromatogram, or if only a part of the chromatogram is displayed (zoom), the number of points contained in this part of the signal.

User name zone: Displays the name of the current user.

Group-project zone: Displays the group and the project names of the current session. In the case of an "all projects" connection, only the name of the group is displayed.

Method Name: If a chromatogram is opened, an additional field mentioning the name of the last method used to process the chromatogram is added after the Group/project.

Waiting process: Indicates the number of processes that have to be performed, or the last process done.

These different fields can be empty, according to the tab selected (Data, Systems, Calibration), the process running or the selected object.

The Shortcuts

Many shortcuts have been defined within CompassCDS, which will be helpful in order to work quickly using the keyboard.

Note that these shortcuts are also displayed within CompassCDS menus.

Warning: The numbers used in the shortcuts cannot be entered from the numeric keypad on the keyboard.

Displaying

The following shortcuts keys of the software are listed below:

F1	Press this key to display the online help menu.
F2	Press this key to display the chromatogram properties in which the sample mass the internal standard quantity and all the global variables (including user input variables) are displayed and can be modified.
F3	Press this key to display the workspace in order to change the full scale or zoom within the chromatogram.
Ctrl+F3	Press these keys to display the peak properties displaying some peak variables.
F9	Press this key to display the Data of the browser window (the panel where the acquired chromatograms, the methods and the sequences are displayed).
F10	Press this key to display the System of the browser window that contains the actively running acquisitions. If this button is pressed in the System panel, the buttons Systems and By type will be selected one after the other.
F11	Press this key to display the Calibration of the browser window, when the calibration curve is displayed. If this button is pressed when a calibration curve is displayed, the buttons Cur, Arch/compound and Arch/date will be selected one after the other.

Run

The following shortcuts quickly perform certain actions:

F5	Press this key to start the integration and the identification of the selected chromatogram.
F6	Press this key to open the Reprocessing window.
F8	Press this key to open the Quick Start window.
Ctrl+Alt+4	Use these keys to start a sequence.
Ctrl+Alt+5	Use these keys to start a reprocessing list.

File

The following shortcuts provide rapid access to certain actions available in the file menu:

Alt+F4	Press these keys to quit CompassCDS Chromatography Data System.
Ctrl+F4	Press these keys to close the selected chromatogram
Shift+Ctrl+F4	Press these keys to close all the files opened in CompassCDS Chromatography Data System
Ctrl+S	Press these keys to save all the files opened in CompassCDS Chromatography Data System
Ctrl+P	Press these keys to print a report for the selected chromatogram with the report style selected in the method.
Alt+Ctrl+F4	Press these keys to display a preview of the report for the selected chromatogram
Ctrl+H	Press these keys to view the chromatogram.
Ctrl+W	Press these keys to access the report style open file box.

To open, close, save, or create a new file, use the following shortcuts:

Ctrl+1	Press these keys to access the chromatogram open file box.
Ctrl+2	Press these keys to access the method open file box.
Ctrl+3	Press these keys to access the calibration curve open file box.
Ctrl+4	Press these keys to access the sequence open file box.
Ctrl+5	Press these keys to access the reprocessing list open file box.
Ctrl+6	Press these keys to access the summary report open file box.
Ctrl+7	Press these keys to access the spectral library edition window (available if you have a Diode Array Detector).

To create a new file, use the Ctrl+Alt keys plus the number defined above. Note that it is not possible to create a new chromatogram or a new calibration curve.

To save files, use the Shift+Ctrl keys plus the number defined above.

To save a file under a new name, use the Shift+Ctrl+Alt keys plus the number defined above. Note that it is not possible to save a chromatogram or a calibration curve under a new name.

To close files, use the Shift+Alt keys plus the number defined above.

Result

The following shortcuts will display the results of the selected chromatogram:

Ctrl+M	Press these keys to display the manual operation history.
Ctrl+A	Press these keys to display the peak result table.
Ctrl+U	Press these keys to display the group result table.

Annotation

The following shortcuts will modify the chromatogram displays:

Ctrl+Alt+C	Press these keys to open the chromatogram annotation screen in order to modify all the chromatogram annotations (Including the following ones).
Ctrl+Alt+E	Press these keys to modify the integration events display within the chromatogram.
Ctrl+Alt+K	Press these keys to modify the peak annotations display.
Ctrl+Alt+I	Press these keys to display or hide the peak identification windows.
Ctrl+Alt+M	Press these keys to display or hide the peak markers.
Ctrl+Alt+N	Press these keys to display or hide the peak annotations.
Ctrl+Alt+B	Press these keys to display or hide the baseline.
Ctrl+Alt+V	Press these keys to display or hide the integration event markers.
Ctrl+Alt+T	Press these keys to display or hide the integration events.

Method

The following shortcuts are used to display different parts of the method.

F7	Press this key to display the Variable editor.
Ctrl+L	Press these keys to display the control method section.
Ctrl+Q	Press these keys to display the acquisition method section.
Ctrl+N	Press these keys to display the pre-processing method section.
Ctrl+I	Press these keys to display the integration method section.
Ctrl+K	Press these keys to display the peak identification method section.
Ctrl+G	Press these keys to display the group identification method section.
Ctrl+B	Press these keys to display the calibration method section.
Ctrl+T	Press these keys to display the suitability tests.
Ctrl+F	Press these keys to modify the peak report, group report and chromatogram formats.
Ctrl+E	Press these keys to display the export method section.
Ctrl+F	Press these keys to modify the peak report, group report and chromatogram formats
Ctrl+O	Press these keys to display the post-processing method section.
Ctrl+R	Press these keys to display the printing method.
Ctrl+Y	Press these keys to display the summaries method.

Sequence and Reprocessing List

Ctrl+↵ (enter) Press these keys to display the information available with the ··· button.

File Structures

There are several different file types used in CompassCDS (chromatogram, method, sequence, etc.). Most files can be opened and displayed using the browser.

Chromatograms

A chromatogram consists of:

Raw data: The acquisition data points.

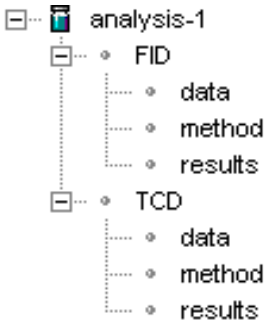
Method: Indicates which is the last method used to process the chromatogram. Control and acquisition methods are never modified during a reprocessing; they are defined at the time of acquisition.

Results: The results group, peak tables and the manual modifications list, if any.

Audit Trail: Traces the history of all methods, which have been used to process the chromatogram and the associated results.

After the chromatogram acquisition, the user can modify its method (integration parameter, identification…) and recalculate the results using these new parameters. The previous method will be kept in the archive, and the new, updated method will be saved. It is also possible to reprocess a chromatogram with a totally different method (Menu option PROCESSING / REPROCESS).

One data file (XXX.DATA) is created by injector, which means that if the chromatographic system is defined with two injectors, two data files are generated by analysis. If several channels are defined by injector, the chromatogram data files generated are composed of several signals. The following picture represents the display of the chromatogram in the browser, in the case of a system with two channels.



Methods

A method consists of several sections:

Control method: Contains the parameters used to execute the acquisition: acquisition rate, start mode and, in the case of a fully-controlled system, the configuration parameters and programs of the chromatograph modules.

Acquisition method: The default parameters will be automatically displayed in the acquisition screens (Quick Start and sequence): run time, run name, etc. It is possible to modify these parameters for every acquisition using these screens.

Preprocessing method: This section contains the blank chromatogram, if any.

Integration method: List of the automatic integration events and the parameter set times

Identification method: The identification parameters of the peaks and groups.

Calibration method: This option is used to set the quantification parameters (Response percentages, external standard etc.) and also to set the calibration curve parameters, if any.

Formats: This feature enables definition of a format for group reports, peak reports, and chromatograms. Formats can also be defined in the properties: right click in the chromatogram, peak or group report and then select the PROPERTIES option.

Export method: The nature, name, path, and content of the method file, which will be exported during the reprocessing is defined.

Suitability tests: This section allows the setup of suitability tests on the defined variables. If one of the tests fails, CompassCDS will display on the screen and/or print in the report, the warning message as defined by the user.

Post processing: Used to run programs or macros after the completed processing of the chromatogram. Be careful to close the files containing the macros before launching them or processing will not be possible.

Print method: Displays the name of the report style.

Summary: Displays the summary or the summary name(s) selected.

File Management

There are two ways to manage the files: using the FILE menu or the File toolbar:

File Menu

Creation of a New File

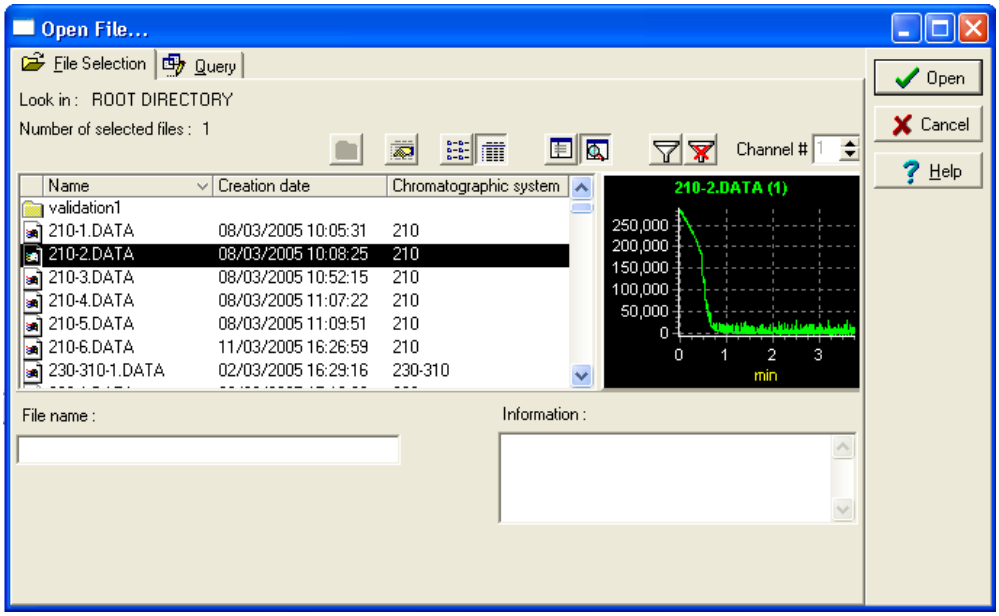
Use the pull-down menu option FILE and then select NEW / NEW METHOD, NEW METHOD FROM TEMPLATE, NEW REPORT STYLE, NEW SEQUENCE, NEW REPROCESSING LIST, or NEW SUMMARY REPORT, to create the corresponding new file in CompassCDS.

For each type, wizards will guide the user through creating the new file.

Open a File

The menu options FILE / OPEN will open the chromatograms, method, report style, calibration curve, sequences, reprocessing lists, summary report.

Each file uses its own “open file” dialog boxes, all based on the same template.



The Open file dialog displays the list of those files visible in the directory associated with the group (when the user is logged on to “All projects") or with the project (when the user is logged on to a specific project).

It is possible to access the sub-directories: double-click on the folder icon ( ). While in the sub-directories, the path is displayed at the top of the window (‘look in :’). It is possible to return to the previous directory by using the root directory button .

NOTE: The Chromatogram open file box allows the user to open chromatograms generated by different software’s: CompassCDS (.DATA) and also AIA (.CDF) files.

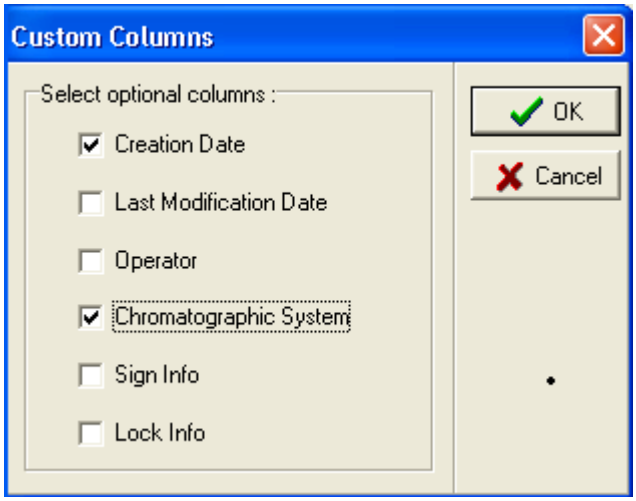
Open file toolbar:

	Use this button to return to the root directory.
	Use this button to customize the columns to be displayed.
	Use this button to display only the list of the files.
	Use this button to display the files with details (acquisition date), etc.
	Use this button to display only files.
	Use this button to display files and a preview of the selected file (only for chromatograms).
	Use this button to apply the filter defined in the Query page
	Use this button to deactivate the filter.

Sorting files

It is possible to sort files by name or creation date in either increasing or decreasing order by clicking in the column header. A down arrow indicates that the files are sorted in increasing order, while an up arrow shows that the files are sorted by decreasing order.

It is also possible to display and to sort files according to other criteria: click on the custom column button , the following window is displayed



User puts a checkmark into the columns to display: creation date, last modification date, operator, chromatographic system, sign info, or lock info associated with the files. The sign info and lock info are available only for chromatograms and inform user that the file has been signed off and locked.

The Open file box size is adjustable, to allow the viewing of all the columns.

NOTE: The creation and modification date correspond to Windows date. For example, if you overwrite a file (when you have the right to overwrite existing files) the creation date is not updated and will correspond to the date of the first creation with the same name.

Selecting file:

To scroll through the file list, use the keyboard arrows or the cursor on the vertical scroll bar.

The selected file is displayed in "BLUE" and, at the same time, a compressed image (if possible) of the file and file information appears at the right of the window. The content of this information is entered during file creation (New method, New sequence). For chromatograms, the information has to be entered in the "Quick Start" window or in the sequence. This field is also accessible when processing a "Save as" file.

To select or deselect several files at the same time, use the SHIFT or Ctrl keys combined with left mouse clicks, as in Windows Explorer. When all the files to be opened are selected, press the OK button.

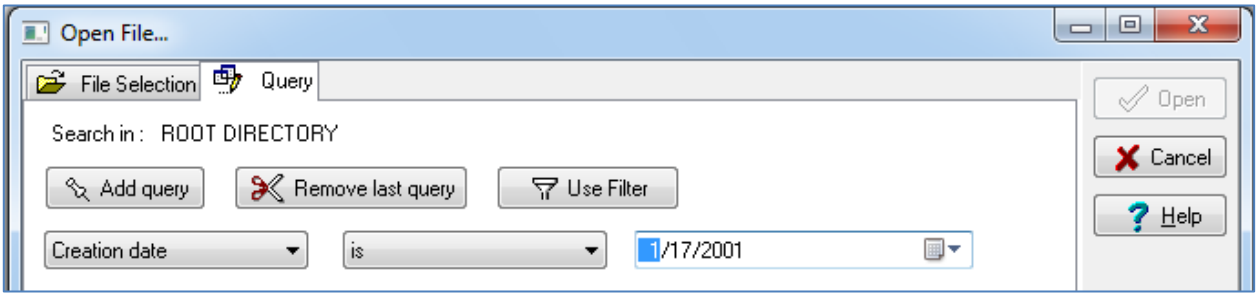
NOTE: It is not possible to open several methods, summary reports or calibration curves at the same time.

Chromatogram preview

If a preview of the chromatogram is displayed in the Open file window, it is possible to zoom in on this image, and magnify it using a click and drag with the left mouse button from the top left-hand corner to the bottom right-hand corner of the area. It is also possible to scroll the zoomed area by holding down and then moving the right mouse button. To zoom out, click and drag the left mouse button from the bottom right-hand corner to the top left-hand corner.

Queries

The Query page allows user to define filters. Once a filter is activated, only the files which correspond to the query's specific criteria are displayed in the File selection page.



Several queries can be made simultaneously. To add a query, click on the Add Query button. To remove the last query, click onto the remove last query button. To apply queries, click onto the Use filter… button. Queries are connected by the 'AND' logical operator, that means all the defined queries must be satisfied to select a file.

Files can be sorted according to:

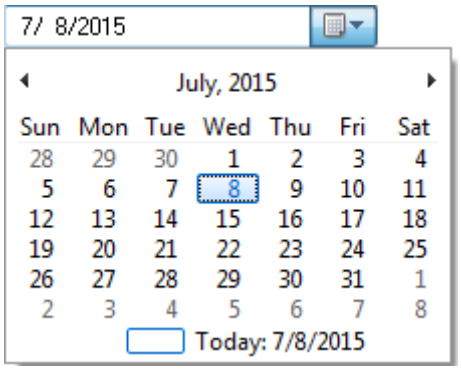
- Acquisition date
- Last modification date
- Operator name
- Information content
- Chromatographic system name associated to the file
- Sign info
- Lock info

The options for the second and third fields depend on the query being specified.

Sort according to dates:

The second field options are:

- is
- is before
- is after
- the date choice is made by activating the third field:



Sort according to: operator name, information field, chromatographic system name:

The second field options are:

- is (this option is not available for information field)
- contains
- begins with
- ends with

The user enters the desired text in the third field.

Sort according to sign info and lock info:

The second field is set to 'is'.

The third field options are: signed file / unsigned file and locked file / unlocked file.

To view the result of the queries, click on the Use Filter… button, the 'File selection' tab is then displayed, listing the files which satisfy the queries. To cancel queries, click on the deactivation icon filter . To again apply the queries defined in the 'Query' tab, click on the use filter icon .

Note that to sort files faster, the user can enter in the 'File name' field of the main screen: The first letters of the file name to open: only files whose name begins by those letters are displayed.

- *letters: only files whose name ends by these letters are displayed.
- *letters*: only files whose name contains these letters are displayed
- *.XXX: only files whose extension is XXX are displayed (only for chromatogram file, allowing the opening of .DATA, .CDF files)

Save a file

Two possibilities exist: save a file with same name (overwriting the previous one) by using the menu FILE / SAVE / SAVE file type, or save the file with another name by using the menu

FILE / SAVE AS / SAVE / file type AS. In both cases, the CompassCDS Chromatography Data System prompts to save the file type corresponding to the active file.

When several files of the same type are opened, the currently selected file will be saved. Therefore, click first on the file to be saved in the browser, then select FILE / SAVE / SAVE file type.

Each file uses its own 'SAVE AS file' box, based on the same template. The Save file window displays a list of the files already created in the directory associated with the group (when the user is logged on to "All projects") or with the project (when the user is logged on to a specific project).

It is possible to access the sub-directories by double-clicking on the corresponding icon ( ). Once in the sub-directory, the path is displayed at the top of the window ('Look in :') and it is possible to return to the previous directory using the Root directory button .

Enter the name of the file in the File Name part. Enter the corresponding information in the corresponding zone and then press the Save button.

Selecting an existing file name will overwrite the existing file. An on-screen warning message will appear since the file that is about to be overwritten will be lost and unrecoverable.

For Chromatogram file, two saving functions are available: 'save method as', allowing to save the chromatogram method as a separate file (.METH) with another name than the one of the method

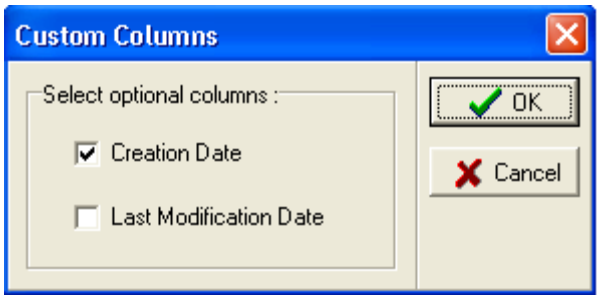
associated to the chromatogram; ‘save method’ allowing to overwrite the method associated to the chromatogram.

File/Save Toolbar

	Use this button to return to the root directory.
	Use this button to customize the columns to be displayed
	Use this button to display only the list of the files.
	Use this button to display the files with details (acquisition date).

It is possible to sort files by name or creation date in either increasing or decreasing order by clicking in the column header. A down arrow indicates that the files are sorted in increasing order, while an up arrow shows that the files are sorted by decreasing order.

It is also possible to display and to sort files according to other criteria: click on the custom column button , the following window is displayed:



The user puts a checkmark into the columns to display: creation date or last modification date.

NOTE: The creation and modification date correspond to Windows date. For example, if you overwrite a file (when you have the right to overwrite existing files) the creation date is not updated and will correspond to the first file creation.

The menu options FILE / SAVE ALL will save all the files that are opened in CompassCDS.

Close a File

The FILE **/** CLOSE / CLOSE Type of file to close menu is active only if a file of this type is currently opened in CompassCDS.

When several files of the same type are opened, the currently selected file will be closed. Therefore in the browser, first click on the file to be closed, then select FILE / CLOSE / CLOSE type of file.

The option to close several chromatograms at the same time is available. Therefore, when choosing the menu option CLOSE CHROMATOGRAM, a window is displayed, which lists the names of all open chromatograms. Select each of the chromatograms to be closed, then press OK. All of the selected chromatograms will be closed at the same time. It is also possible to select or deselect all of the chromatograms using the Select all button.

The menu option FILE / CLOSE ALL will close all of the files that are currently opened in CompassCDS.

Competitive File Access

If a user tries to open a file which is already opened in CompassCDS by another person, a message advises the user that the file can only be opened in read-only mode. No modification can thus be saved, therefore the Save button of a read-only file is inactive.

Chromatogram: A read-only chromatogram can be modified either by the "Integrate" (F5) function or by manual integration or identification, but it cannot be saved. CompassCDS allows the printing of the modified results. A report corresponding to an unsaved data file is printed with a "Data Not Saved" background.

Method: A read-only method can be modified but not saved.

Sequence: When a sequence is in read-only mode, only column customization and sequence printing are allowed. Other modifications are not allowed (add/delete lines, clear sequence, start sequence…)

Reprocessing list: When a reprocessing list is in read-only mode, only column customization and reprocessing list printing are allowed. Other modifications are not allowed (add/delete lines, clear reprocessing list, start reprocessing list…)

Summary report: When a summary report is in read-only mode, it can be printed, but the chromatogram number and variables cannot be modified.

Report style: A read-only report style can be modified, but not saved.

Calibration curve: A message advises the user when the curve is already use by another user.

Generally speaking, when a file is already opened, CompassCDS forbids the creation of a new file with the same name.

The "Save as" function also forbids to keep the same name. But, chromatogram method can be saved with the same name if the "Save chromatogram method" CompassCDS Configuration Manager profile has been selected. Select the "Save chromatogram method" from the popup menu of the chromatogram method in order to save the chromatogram method under the same name.

File Toolbar

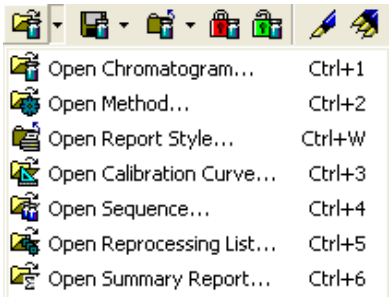
The icons also provide chromatogram management as in the corresponding menus. The only difference is that the icons provide faster access.

The first icon will open files, the second will save current files, and the third will close files.

The graphic appearance of the toolbar (three first buttons) changes slightly according to the active file type currently loaded in CompassCDS. For example, if chromatograms are being managed, the open file icon will appear as . If methods are being managed, the icon will appear as . When working with sequences, the icon will appear as with calibration curves, the icon will appear as .

When working with the reprocessing list, the icon will appear as .

If the current icons are displayed for chromatogram management, it is possible to change this display. For example, to open a calibration curve, click on the arrow at the icon's right, then select the correct sub-menu:



The appearance of the toolbar is changed when a file is opened, saved, closed, or when a file is selected.

File Storage and File Extensions Generated by CompassCDS

Files are stored in directories whose paths are defined in CompassCDS Configuration Manager.

Each file type generated by CompassCDS uses its own extension, thus making it easy to find using the Windows Explorer.

- Chromatogram: .DATA
- Method: .METH
- Sequence: .SEQU
- Reprocessing list: .REPL
- Report style: .STYL
- Method report style: .STYM
- Calibration report style: .STYC
- Calibration curve: .CALB
- Summary report: .SUMR

The following characters are not allowed in a file name \ / : * ? " < >.|

The chromatograms, methods, sequences and reprocessing lists files are stored in the project root directory. Calibration curve, summary report and report style files are stored in the group root directory, thus allowing their use in several projects belonging to the group.

If a method is defined in a project, and that user wants to use it in another, the user must save it "as a template method" and once logged in the right project, the user must create a "new method from template" (see page109). It is recommended that the user refrain from copying a method from a directory to another. Indeed since, a method is linked to a project at its creation. All chromatograms acquired with this method are stored in the project directory. Copying this method in another project directory, via the Windows Explorer, will introduce confusion; all newly acquired chromatograms will be stored in the original project directory and not in the new one. Nevertheless, calibration curves and report styles can be copied from one group to another and chromatograms from one project to another as well.

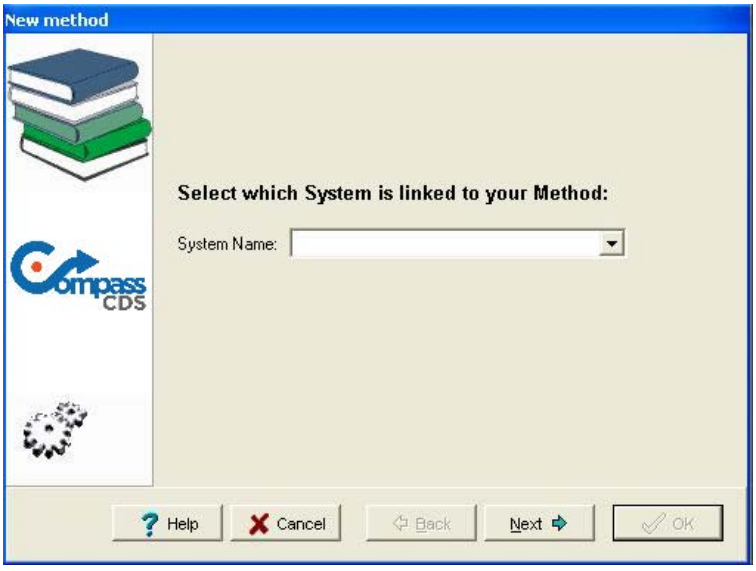
The Method

The method contains parameters for instrument control, data acquisition, chromatogram processing, and the format of results.

It is not compulsory to define all of the method sections when initially setting up an acquisition, but it is mandatory to complete the instrument control section prior to start an acquisition (especially for an automatic operation).

Create a Method

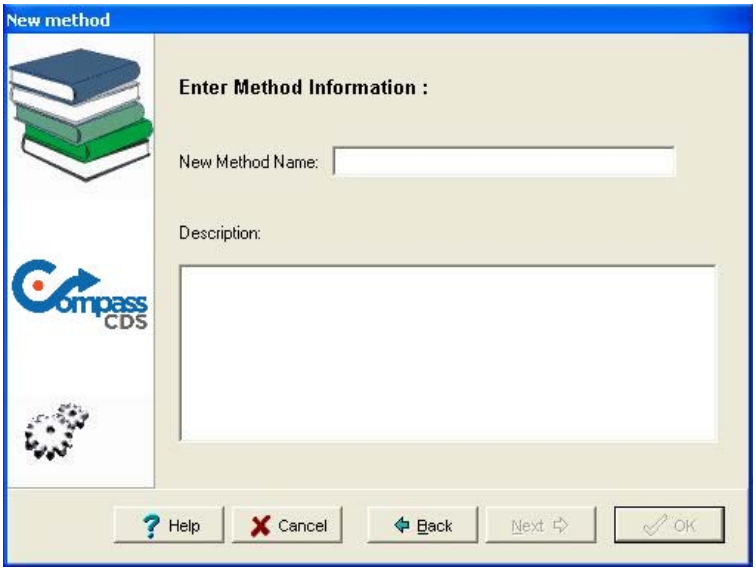
Select the FILE / NEW / NEW METHOD options from the main menu. A wizard provides assistance during the first steps of method creation:



Choose the system (chromatograph) associated with the method. A method is created for a particular system. Thus, when starting an acquisition, the name of the system that performs the acquisition must be correct, since method access is limited only to those associated with this system.

NOTE: If the user is connected under 'all projects', the 'New method' wizard will contain one additional field to allow selection of the project.

Once these two fields are completed, the NEXT button is activated. Click on the NEXT button to move to the second step of the method creation:



Enter the new method name in the first edit box. In the description box, enter information concerning the method (optional). This will be displayed in the open file window, when the file is selected.

Once the entry of these two fields is completed, the OK button is activated. Click on the OK button, and the new method is created and will be opened with default parameters in CompassCDS.

The next step is to define each of the method sections. The instrument control section must be defined in order to start an acquisition. This is the minimum requirement. However, the other sections may be defined later, after the acquisition of a chromatogram in order to view the peak retention times.

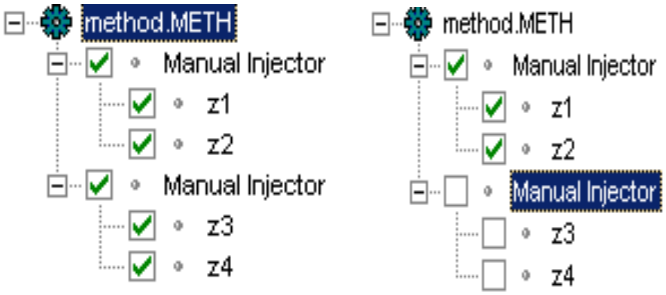
For multi injector system:

Control section is defined for the whole system. Only one control method must be defined.

Acquisition section is specific for each injector.

Other sections of the method (Pre-processing, Integration, Identification…) are specific to each detector. Parameters must be set for each detector channel.

It is possible to disconnect an injector, or channels, by unchecking them in the browser.



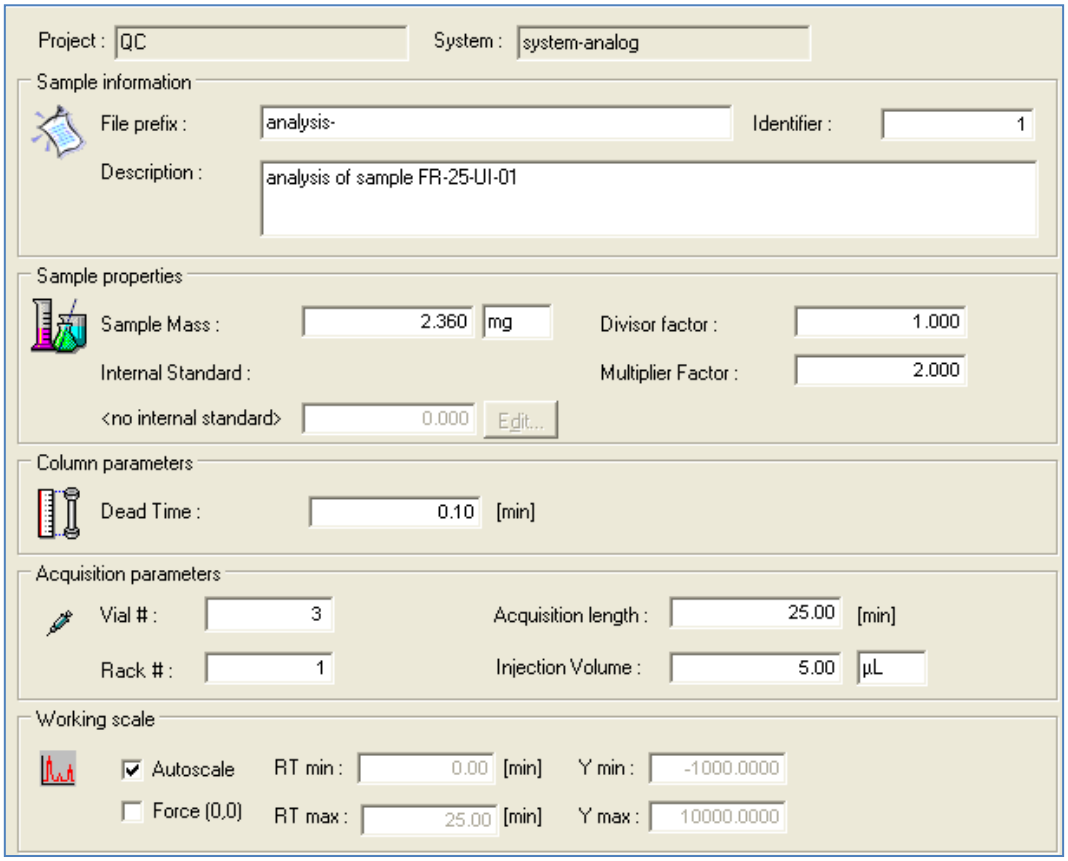
The Different Parts of the Method

Control

This section of the method depends on the chromatographic system. For fully controlled instruments (e.g., where a specific instrument control driver is used), the control section consists in all the parameters that can be set for this chromatography system.

Acquisition

In the acquisition method, default parameters are set as they will be displayed in the acquisition windows: Quick Start or sequence. It is also possible to modify these parameters before starting the acquisition.



File prefix: Specify the first part of the chromatogram name in this zone. The chromatogram name will have the identifier appended to it.

Identifier: Specify a numeric value for the second part of the chromatogram name in this zone. For example, if the file prefix is ‘Run’ and the identifier is 55, the name of the chromatogram will be Run_55.data. The identifier is incremented automatically after each acquisition in the case of single acquisitions (started using the Quick Start).

Description: Information about the run may be entered in this area. This information will be saved with the chromatogram and displayed in the open file window and in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES). The description can be a maximum number of 255 characters.

Sample mass: Enter the total mass of the sample in this field. This value can be used for the calculation of compound amounts. The sample mass variable can be used along with all the other variables available in the variable editor. Enter the mass unit in the adjacent edit box.

Internal standard: It is possible here to define default internal standard quantity (or quantities). User must previously have defined the name of the internal standard(s) in the Peak Identification part of the method and have indicated which (whose) peak(s) are internal standard(s) in the calibration part of the method. Enter then the corresponding value in the internal standard zone, or if there are several internal standards, press the Edit button.

NOTE: If the internal standard quantity changes from a sample to another, it is not advisable to enter a value at this step. The internal standard can be entered in the Quick Start window, in the corresponding column, in the sequence for an acquisition, in the chromatogram properties for single run reprocessing, or in the corresponding column in a reprocessing list.

Multiplier factor: This variable is used to multiply all the quantities calculated by the same factor.

Divisor factor: This variable is used to divide all the quantities by the same factor.

Specific Channel Parameters: This option is displayed only in the case of a multi-channel system. It allows the user to enter different Multiplier factors, Divisor factors, sample masses and working scales by channel.

Dead time: This time corresponds to the time required for the sample solvent (or any non-retained compound) to reach the detector. This time is used for the calculation of the selectivity and capacity factor.

Vial: The vial number can be entered for information only or can be used to specify which autosampler vial number should be injected.

Rack: The rack number can be entered for information only or can be used to specify the rack number that contains the vial that should be injected in the case of a fully controlled autosampler.

Acquisition length: Specify the total acquisition time in this field.

Injection volume: The injection volume can be entered for information only or can be used to specify an injection volume for the autosampler if fully controlled by CompassCDS. Enter the volume unit in the adjacent edit box.

Working scale: By default, the Y scale of the chromatogram is defined according to the maximal signal. However, in the case of a chromatogram containing a very large solvent peak, it can be useful to display only the small peaks. By un-checking the Automatic Box, it is possible to select limits to display the chromatogram during the acquisition, both on the main screen and in the report (if special limits are not set in the report). The Force (0,0) option forces the scale of the acquisition screen to display the origin (0,0), for example, to show the (offset) of a chromatogram. This function cannot be used to force the signal to go through the origin.

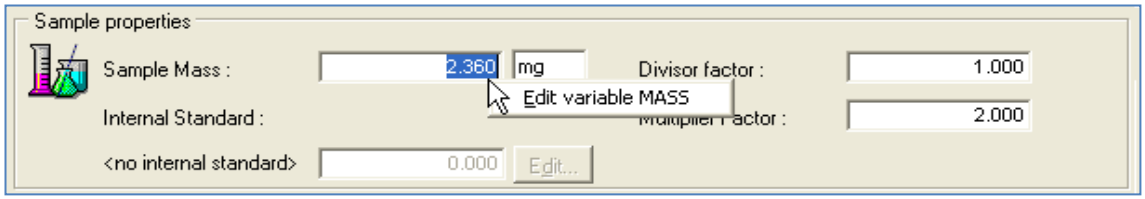
User can easily modify the format of the following displayed variables:

In **Sample Properties:** every variable

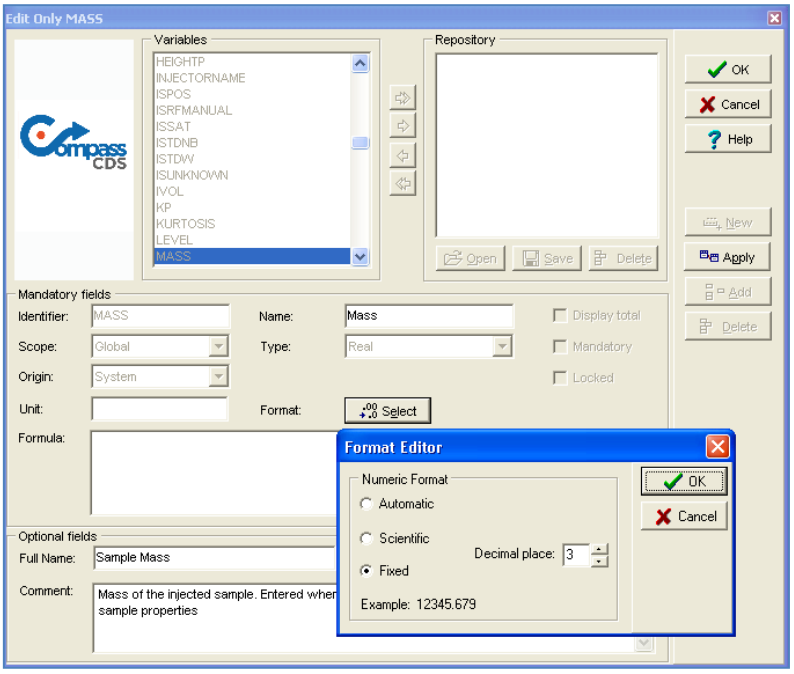
In **Acquisition parameters:** acquisition length

In **Working scale:** RT min and RT max

To change the format, put the cursor of the mouse on the box corresponding to the variable which format has to be modified, click on the right mouse button and select the option ‘Edit Variable XXX’ in the popup menu, where XXX represents the variable name.



The variable screen is then displayed, allowing only the modification of the selected variable format. For example for the sample mass, the following screen is displayed:



Note that the ‘Quick Start’ screen is almost the same as the one of the acquisition section of the method. The format of some variables displayed in the ‘Quick Start’ screen is customizable in the associated method, and NOT modifiable from the ‘Quick Start’ screen.

If using a system with several channels, an additional option is available: Specific Channel Parameters. When this option is checked, some variables usually defined for all channels can be defined by channel. These variables are: multiplier factor, division factor, sample mass and working scale, of course as in the case of non-Specific Channel Parameters mode, internal standard values and User inputs variables remain channel dependent.

If using this option, the user must enter values in each acquisition part of the method of each channel. If not using this option, the acquisition part of the method is common to all channels (of the same injector).

This means that during acquisition (Quick Start or Sequence), different values can be entered for these variables according to the channels.

Pre-processing

Subtract a Blank to a Chromatogram

In the preprocessing section of the method, it is possible to select a blank chromatogram that will be subtracted from the sample chromatogram before any further calculation.

Press the Open icon: and select the blank chromatogram in the Open file window. If the blank chromatogram has been acquired on several channels, the channel to be subtracted must also be selected. The blank must be acquired with the same frequency (number of points per minute) than the one of the original chromatogram.

Subtracting a file of the Same Sequence:

In the sequence, it is possible to define blank files that will be subtracted from the following chromatograms to be acquired. To define a blank sample run, blank must be selected in the sample type column of the sequence.

For example if a sequence consists of ten lines: The first and sixth ones should be blank files and should be subtracted from the second to the fifth and the seventh to the tenth runs respectively. The only operation necessary is to select Blank in the Sample type column for the first and the sixth lines.

Recovering Raw Data:

When a blank is subtracted from a chromatogram, the raw data are not lost: to recover it, delete the blank called in the pre-processing section of the method with the button, and then reprocess (F6) the chromatogram and the raw data are recovered.

Integration

Integration Events

Peak Detection Events

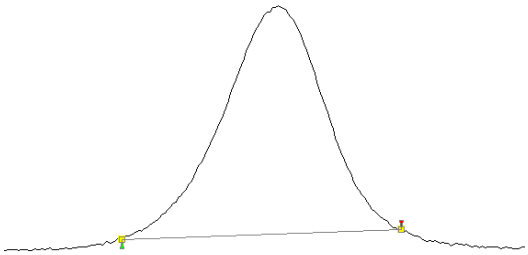
Set peak width

This event defines the width of the peak to be found in the chromatogram. This value is used to smooth the chromatogram by grouping several acquisition points during peak detection. The number of grouped points depends on the chosen width. A point whose height is the mean of all the points in the group represents each group.

Enter a value corresponding approximately to the width of the narrowest peak to be detected in the chromatogram.

If the peak width varies greatly in the same chromatogram, it is possible to change peak widths throughout the chromatogram as necessary. Set new values in Set Peak Width, half it using Half Peak Width, or double it using Double Peak Width.

If the defined peak width value is too small, the peaks will be detected, but too late.



If the defined peak width value is too large, the peaks will not be detected at all.

A peak width must be defined before integrating the chromatogram.

The default peak width is 0.2 minutes.

Set Threshold

This parameter is used to define the start and the end of peaks and eliminates the lowest signal variations due to noise or to detector signal drift.

CompassCDS allows two types of threshold calculation: relative threshold (see page62) or absolute threshold (see page62). The absolute threshold is defined in the METHOD / INTEGRATION / PARAMETERS menu, by unchecking the Use relative threshold option. Details about the way CompassCDS detects peaks are described in the “Peak start and end determination” section (see page62).

If relative threshold is used (by default), the chromatogram is first normalized to 100,000 (Highest peak of the chromatogram) in order to obtain a similar detection from one analysis to another (for example, if the injected quantity varies). If absolute threshold is used, no preliminary calculation is done. Next, the points are grouped depending on the peak width defined above. The mean height of a group of points is compared to the mean height of the following group. If the difference is higher than the threshold, the integrator marks the beginning of a peak. The position of the marker is adjusted by considering only the points. The peak will be kept only if its area and height are larger than minimum values defined by user.

The peak ends are detected in the same way using the threshold.

The value of the threshold is important. If too high of a threshold value is defined, the peak starts will be detected too late and the peak ends too early. Moreover, small peaks could not be detected at all. If a too small of a threshold value is defined, the peak starts will be detected too early, and the peak ends too late, and signal noise can be detected as peaks.

The user can define the threshold value, or CompassCDS can estimate it using Estimate threshold according to the peaks that should be detected.

It is also possible to add a value to the threshold using Add to threshold. For example, if the threshold is estimated at the beginning of the analysis, and the signal noise increases at the end of the analysis, the threshold will need to be increased only at the end. Note that it is possible to add a negative value in order to decrease the threshold value.

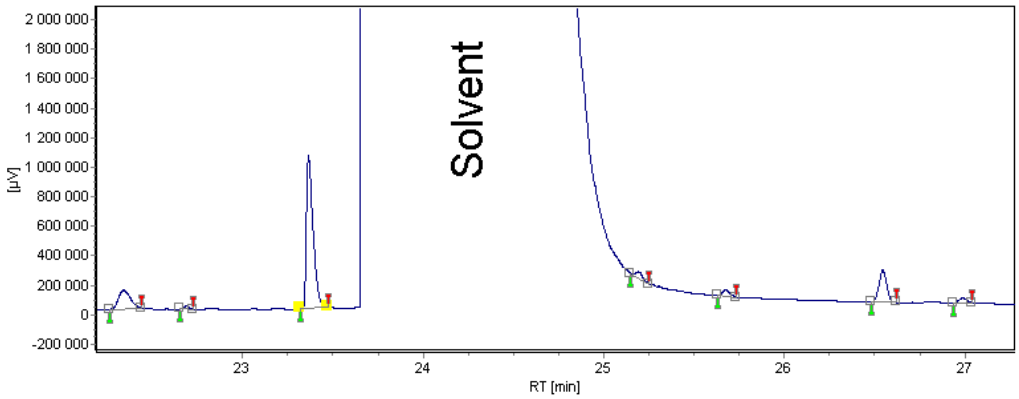
The default threshold value is 10.

Set Solvent Threshold

This event performs the elimination of solvent peak(s) if they are not peaks of interest.

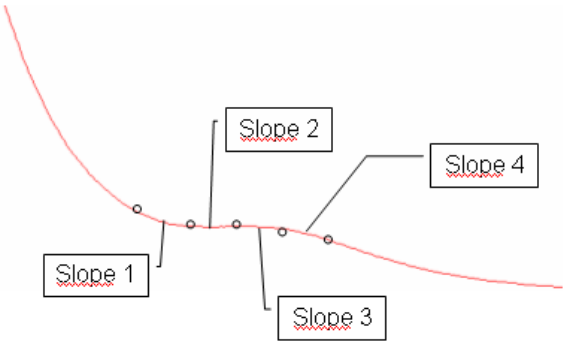
The parameter associated with this event works in a manner similar to the absolute threshold (without previous normalization of the chromatogram). The points are grouped depending on the peak width defined above. The mean height of a group is compared to the mean height of the following group. If the difference is higher than the solvent threshold, CompassCDS considers that the peak is a solvent peak, and does not integrate it.

The defined value must be high enough to prevent the deletion of peaks of interest.



Set Shoulder Threshold

This event allows the user to have a better sensibility for detecting peaks where the peak start cannot be found easily.



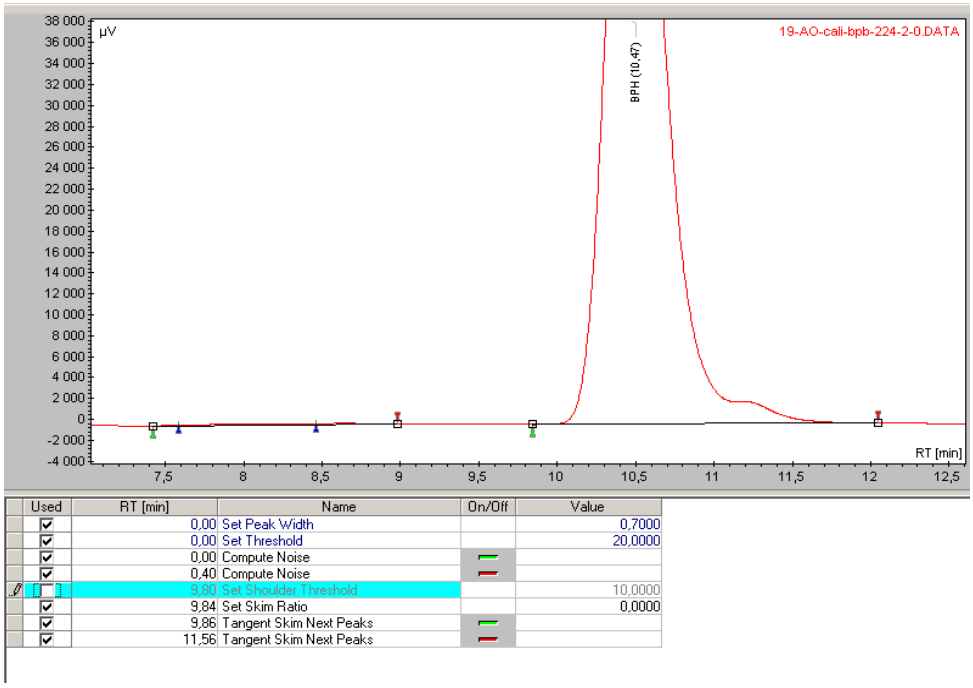
The user has to enter a value for the Shoulder Threshold event. A possible start point is determined between Slope 1 and Slope 2 when:

- |Slope 2| < Shoulder threshold
- |Slope 3| < Shoulder threshold
- |Slope 1| > Shoulder threshold
- |Slope 4| > Shoulder threshold
- Slope1×Slope4>0

NOTE: The slope is computed across the data bunch interval.

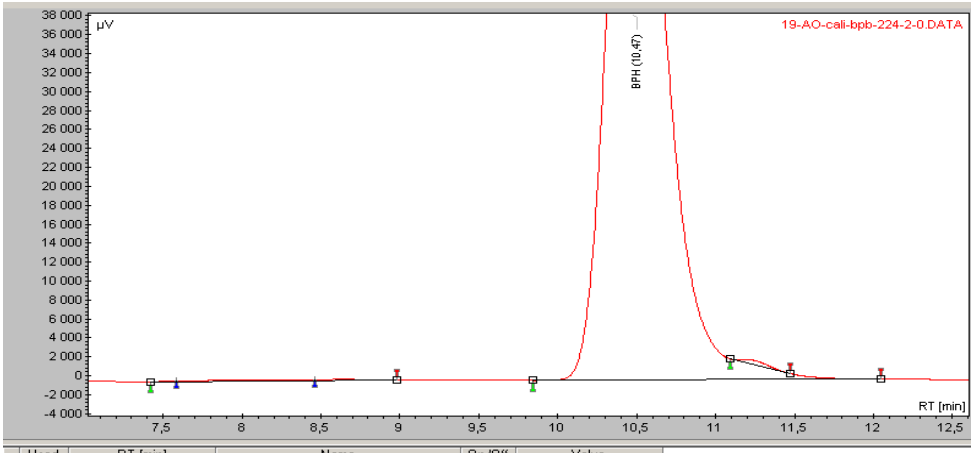
For example,

Before:



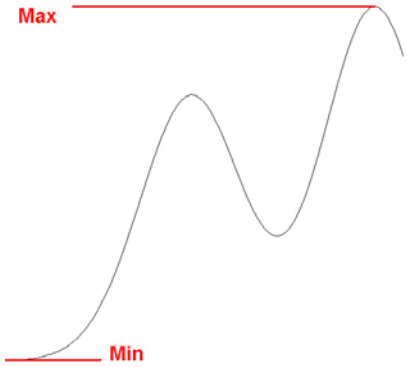
Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,7000
☑	0,00	Set Threshold		20,0000
☑	0,00	Compute Noise		
☑	0,40	Compute Noise		
☐	9,80	Set Shoulder Threshold		10,0000
☑	9,84	Set Skim Ratio		0,0000
☑	9,86	Tangent Skim Next Peaks		
☑	11,56	Tangent Skim Next Peaks		

After:



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,7000
☑	0,00	Set Threshold		20,0000
☑	0,00	Compute Noise		
☑	0,40	Compute Noise		
☑	9,80	Set Shoulder Threshold		10,0000
☑	9,84	Set Skim Ratio		0,0000
☑	9,86	Tangent Skim Next Peaks		
☑	11,56	Tangent Skim Next Peaks		

Max Y threshold %: By default to be integrated, a peak must satisfy the following condition: minimum signal value < 1% of the maximum signal value of the peak. To integrate some peaks that are not integrated by default by the software, user can reduce this value up to 0. In the contrary, to not integrate some noise on the top of a solvent peak for example, user can increase this value.



Estimate Threshold:

If the event "Estimate threshold" is not defined, solvent peaks are integrated. The user can define several events ‘Estimate threshold’. For each time the event is defined, CompassCDS calculates both absolute threshold and relative threshold (see definition in the Integration algorithm section). The calculated values are displayed in the chromatogram properties and are named: AUTOTHRESHOLD_ABS_I and AUTOTHRESHOLD_REL_I, where I represent the I^{th} defined event in the integration table.

Compute noise

This event calculates the noise value from the signal during an acquisition. (The calculations are explained in the standard global variables). The noise needs a start and an end to be calculated: Add a Compute noise ON event at the time when the noise calculation should start, then add a Compute noise OFF event at the time when it should stop. Be careful not to include peaks in the defined area because they would be considered as noise.

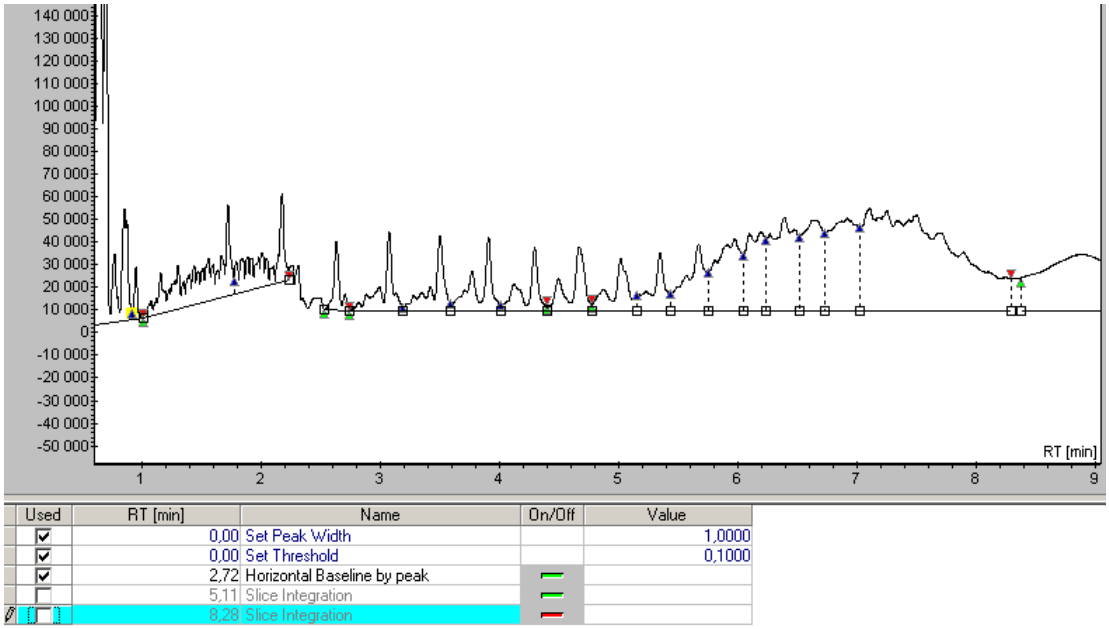
The calculated value is displayed in the chromatogram properties. The corresponding variable is "NOISE". If no time period is defined, the NOISE value is equal to 0.

NOTE: If several events (NOISE ON / NOISE OFF pairs) have been defined, only the value calculated for the last period is displayed.

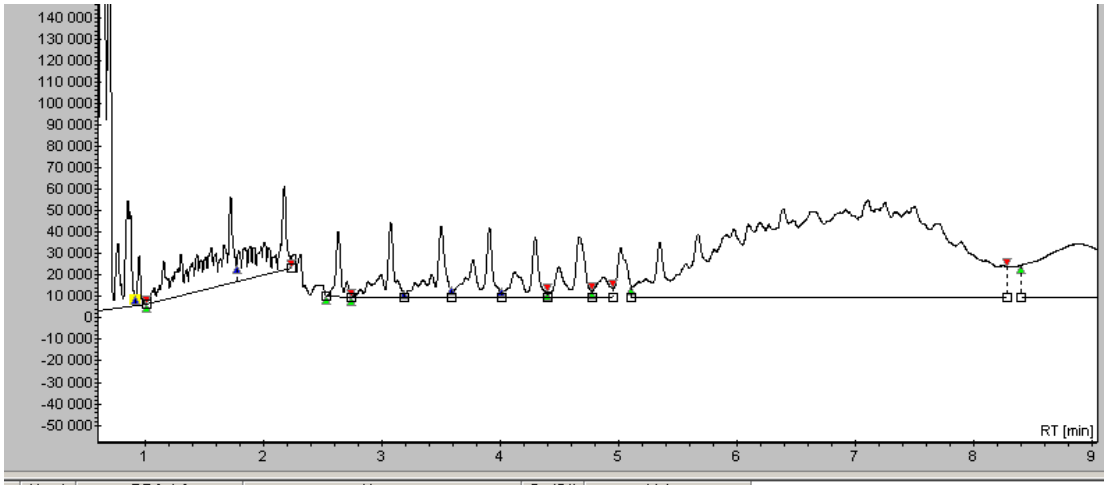
Slice integration:

This event allows the user to deactivate the automatic integration during a defined period. This can be useful to integrate a set of peaks as a single peak. This event is totally independent of the Peak width and the Set threshold.

Example:



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		1,0000
☑	0,00	Set Threshold		0,1000
☑	2,72	Horizontal Baseline by peak		
☐	5,11	Slice Integration		
☐	8,28	Slice Integration		



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		1,0000
☑	0,00	Set Threshold		0,1000
☑	2,72	Horizontal Baseline by peak		
☑	5,11	Slice Integration		
☑	8,28	Slice Integration		

Set Minimum Height/Area

These parameters are used to prevent the integration of noise as peaks or to eliminate small peaks which are not of interest in the analysis.

All peaks whose height or area is less than the minimal height and/or area parameters set are deleted from the peak report. Therefore, choose parameters that are less than the areas and heights of all the peaks to be integrated.

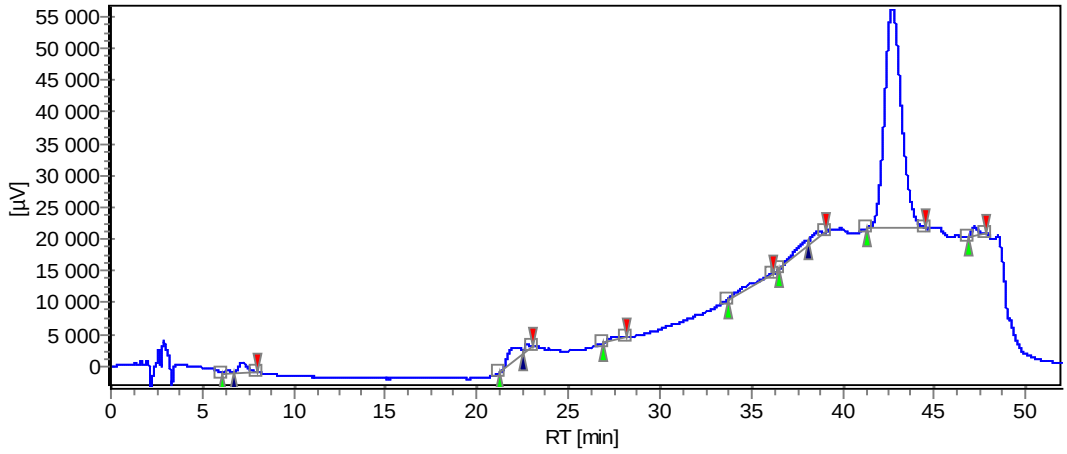
Minimal heights and areas can be defined absolutely or relatively to total chromatogram heights and areas using the events “Set minimum height %” and “Set minimum area %”.

By default, minimum area and height settings are equal to zero.

Forced peaks

Turn integration On/Off

These events activate or deactivate integration within sections of the chromatogram (e.g., during baseline fluctuations (injection shock)):



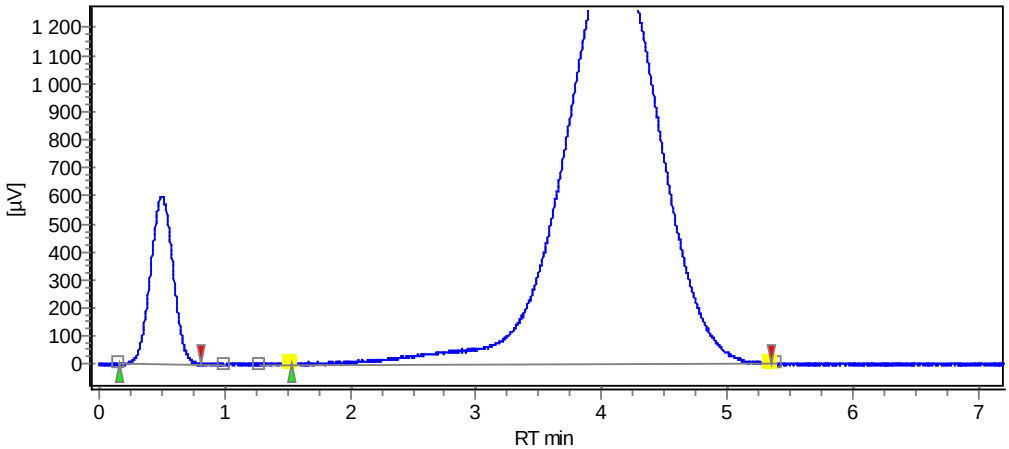
In the above example, integration has been deactivated during the first 5 minutes.

Start/Stop peak now

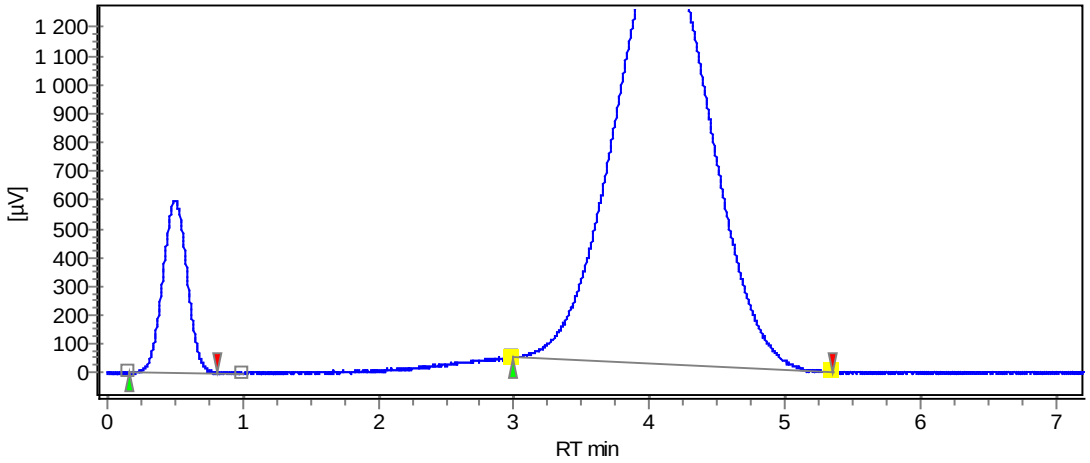
These events allow the start or the end of a peak to be defined, earlier or later, without having to modify the integration parameters. The marker is re-positioned at a new retention time when this event is specified.

For example,

Before:



After:

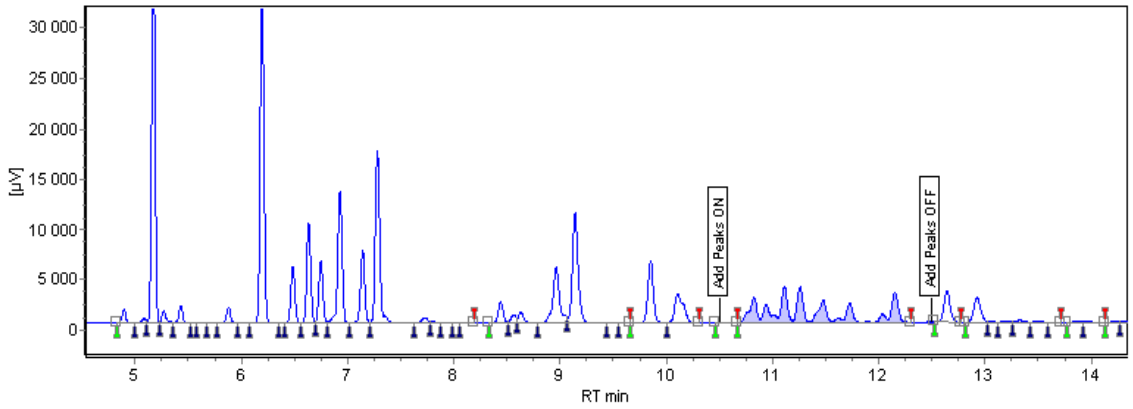


Be cautious if using these events in automatic mode: check that retention times have not shifted from one analysis to another.

Add peaks

This event enables addition of several peaks. All the peaks defined between the activation and the deactivation of this event is grouped into one peak.

For example, isomers whose names are not known peak by peak, but contain nearly the same response factors can be considered as one group. The peak grouping is considered as one peak. Note that the peak start or stop position is automatically adjusted around the defined time to avoid the baseline cut by the signal.



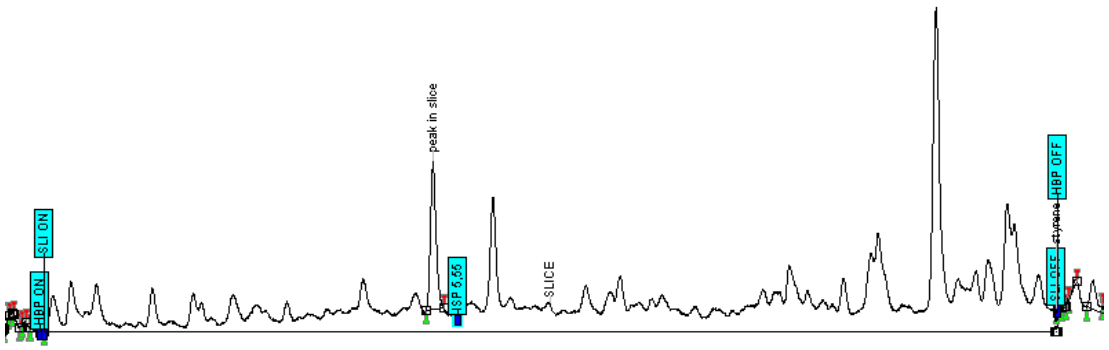
In the above example, the peaks between 10.5 and 12.5 minutes are added.

NOTE: If the baseline cuts the signal in the section corresponding to the ‘Add peaks’ events (ON + OFF), the expected added peak can be not defined. In this case, change the baseline position to the corresponding integration event(s).

In slice peak

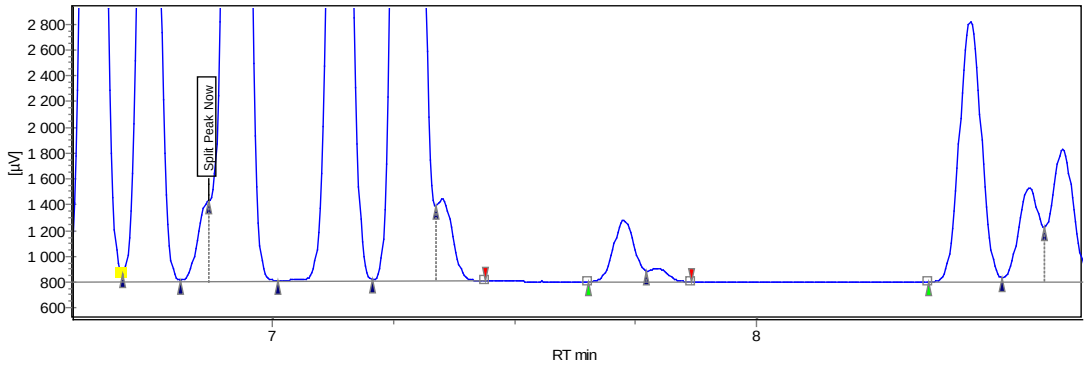
This event has to be used within a slice (between Slice integration ON and Slice Integration OFF integration events). It allows the user to add a peak in a slice. A tangential baseline is drawn between the start peak and the stop peak marker positions, and its area is removed from the slice area.

The In slice peak integration event is defined at a time with a relative windows (in minutes). The software is looking for the highest peak to integrate in the time interval defined by the user [RT± windows].



Split peak

This event will split a peak into two parts, and can be used either to separate peaks poorly resolved or to obtain specific results on parts of some peaks in certain applications.



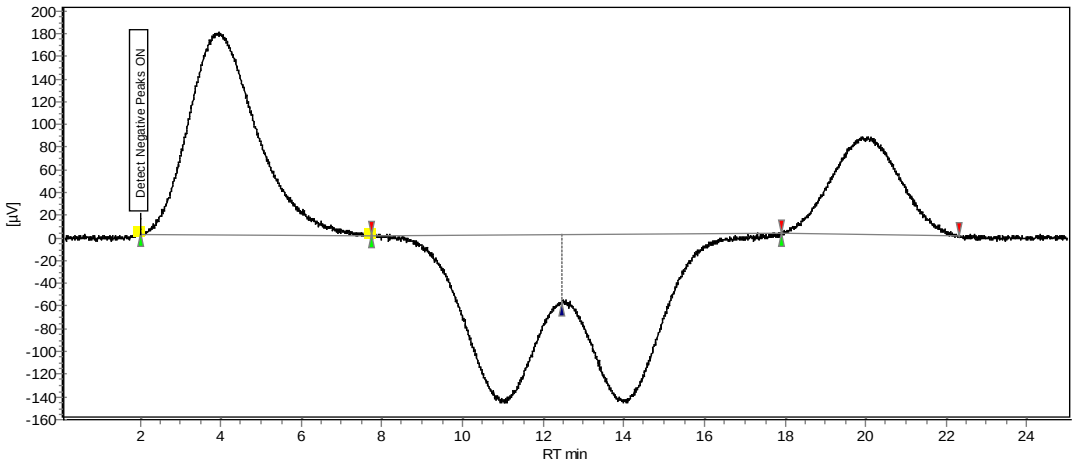
Be cautious when using this event in automatic integration mode. If retention times vary from one analysis to another the results may not be what were expected.

Negative Peaks Processing

The Detect Negative Peaks event activates negative peak detection.

When negative peak detection is activated (On), it is better to also deactivate it, (Detect negative peaks off), because during the integration algorithm the CompassCDS tries to place a baseline between these two events (On and Off). If the signal passes below this raw baseline, CompassCDS searches for negative peaks. When the signal is above this raw baseline, CompassCDS searches for positive peaks.

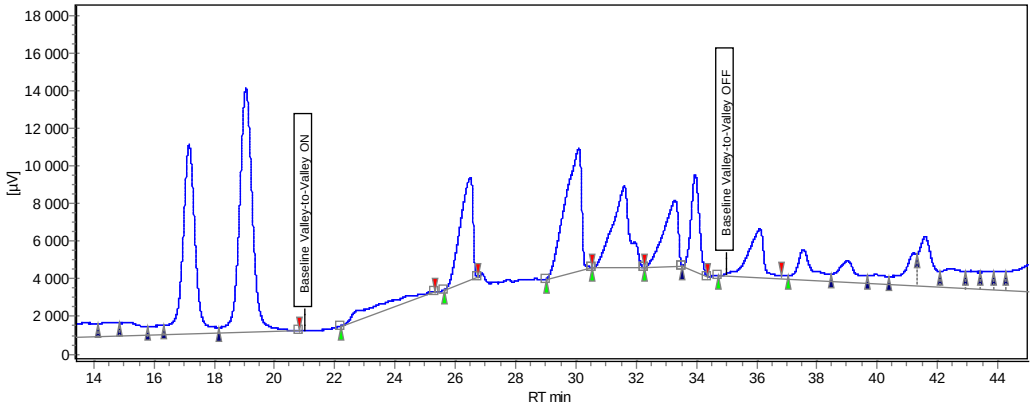
Negative peak detection depends on the signal height when the event is activated and deactivated, so it is also dependent upon the time when the events are specified. As a consequence, be careful to ensure that negative peak detection is not activated or deactivated after the beginning of a peak.



Baseline Processing

Baseline valley to valley On/Off

When this event is activated, the baseline passes through all the valleys.



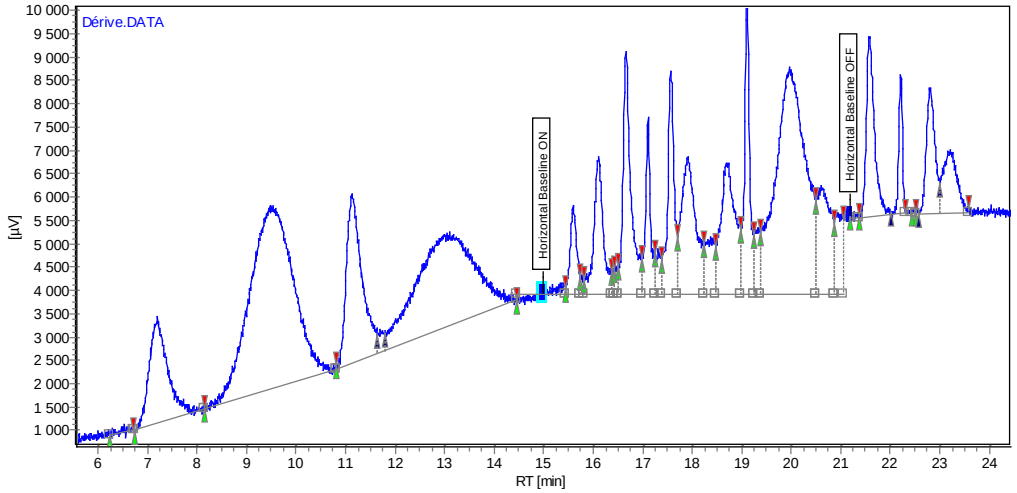
Each peak has its own baseline drawn from the peak start marker to the peak end marker.

Horizontal baseline

This event enables the definition of a horizontal baseline.

A horizontal baseline is drawn from the activation of this event until its deactivation. It is imperative to define the event couple (ON and OFF) to apply this event.

NOTE: ON is symbolized by a green mark and OFF by a red one.

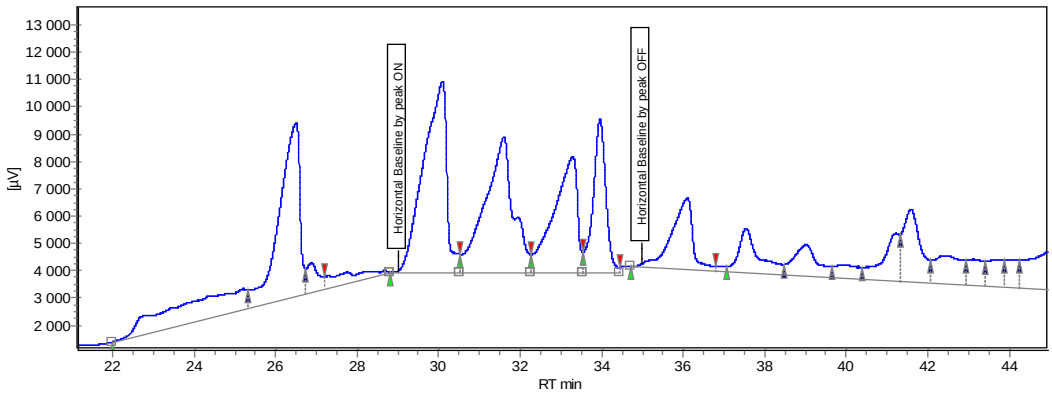


The height of the baseline is the height of the signal when the event is activated.

It is better to use the “Horizontal baseline by peak” event, because the height of the baseline will be related to the start or the end of a peak, and not to the event activation time.

Horizontal baseline by peak

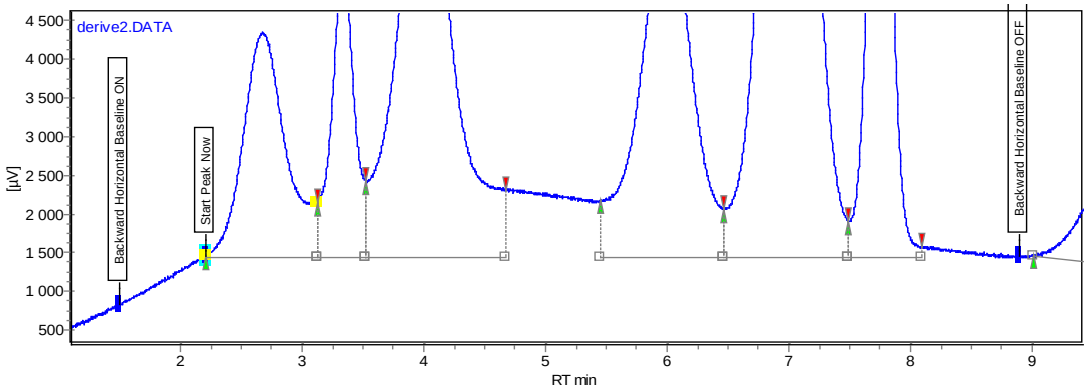
This event enables definition of a horizontal baseline. The horizontal baseline start or stop are not applied to the defined times, but to the nearest start or stop peak time



If an event is activated at the beginning of a peak (between the start marker and the peak apex), it becomes operative at the peak start time. If the event is activated at the end of the peak (between the top of the peak and the stop marker), it becomes operative at the peak stop marker time.

Backward Horizontal baseline

This event enables definition of a horizontal baseline at the level of the signal when this event is deactivated.

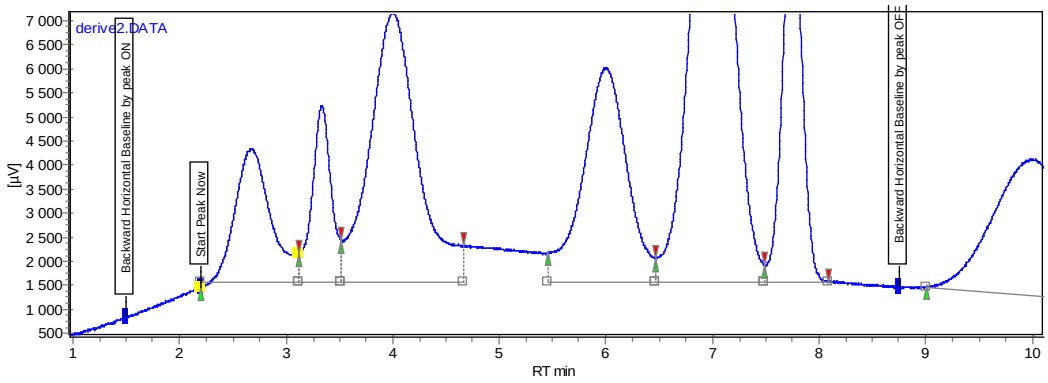


The horizontal baseline is drawn from the activation of the event until its deactivation. The baseline is drawn at the level of the signal when the event is deactivated.

As a consequence, the two events “Horizontal baseline Backward On” and “Horizontal baseline Backward Off” must be defined.

Backward Horizontal baseline by peak

This event enables definition of a backward horizontal baseline. The horizontal baseline is drawn from the activation of the event until its deactivation. The baseline is drawn at the level of the signal at the stop marker of the peak preceding the event deactivation.

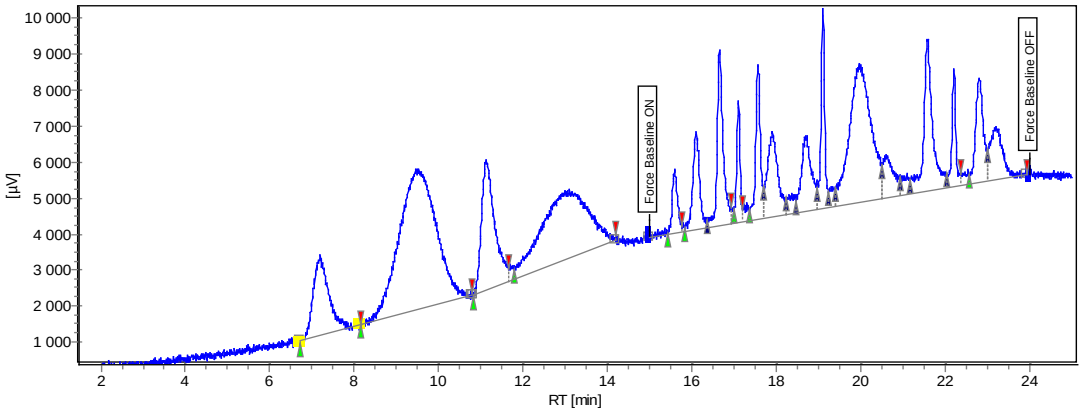


As a consequence, the two events “Backward Horizontal Baseline by peak On” and “Backward Horizontal Baseline by peak Off” must be defined.

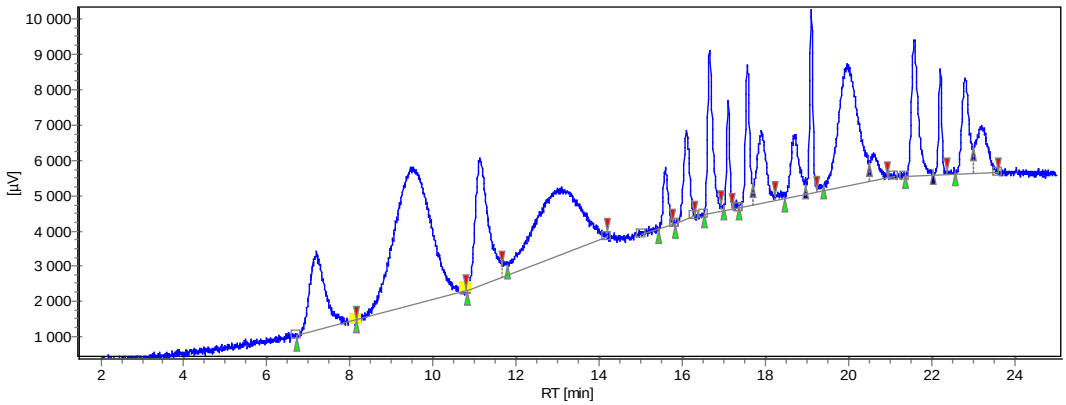
Force baseline

This event forces all the peaks between the events “Force baseline on” and “Force baseline off” to have a common baseline. The peak markers of the first and last peaks are therefore modified by this event. To prevent modification of the first and last peak markers, the recommended event to use is “Force baseline by peak”.

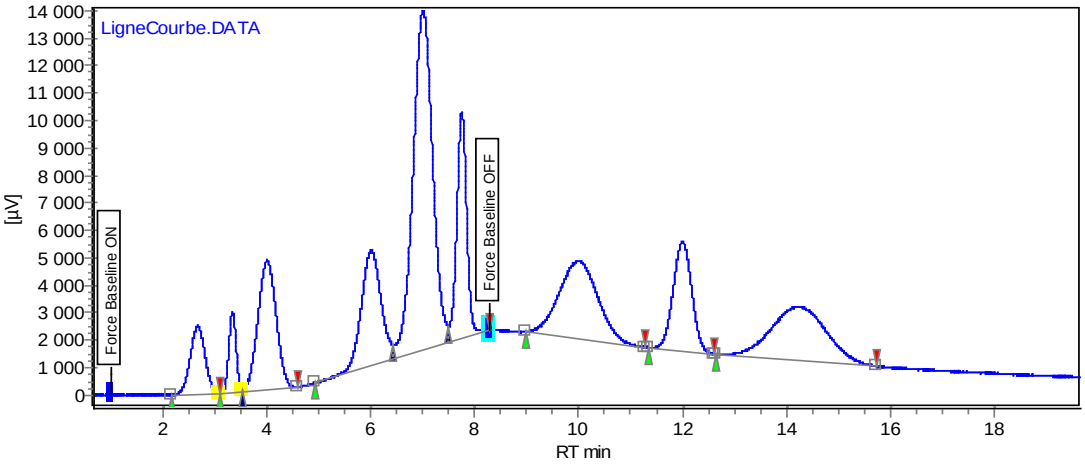
As a consequence, the two associated events “Force baseline on” and “Force baseline off” must be defined.



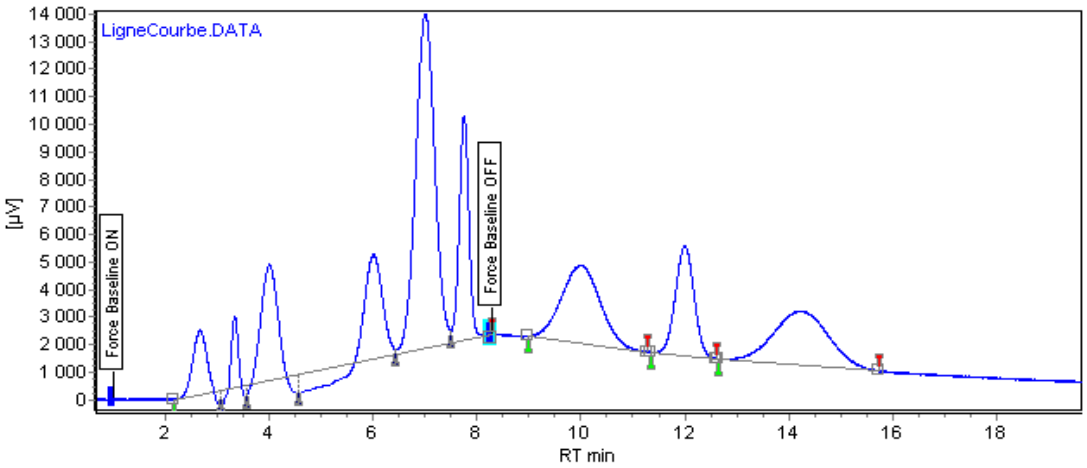
Instead of



If the forced baseline penetrates the signal, the baseline will automatically adjust so that it always remains under the signal.



Instead of



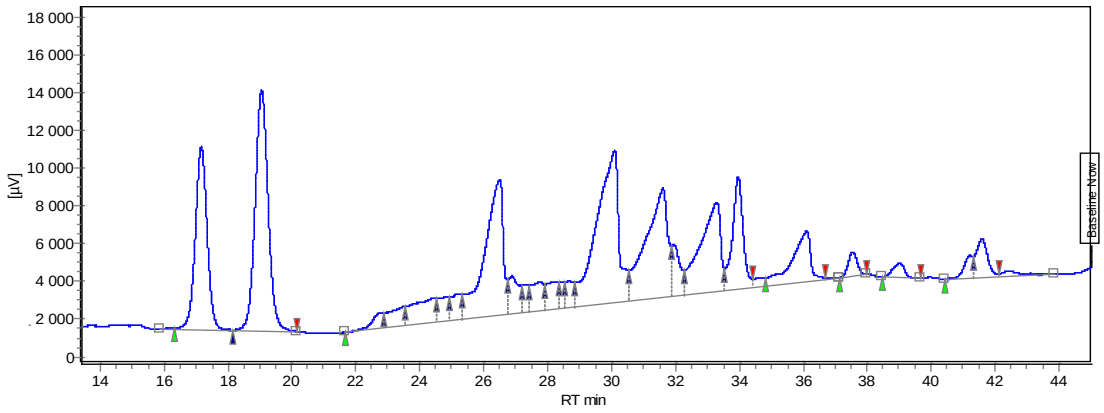
Force baseline by peak

This event forces all the peaks between the events “Force baseline by peak on” and “Force baseline by peak Off” to have a common baseline.

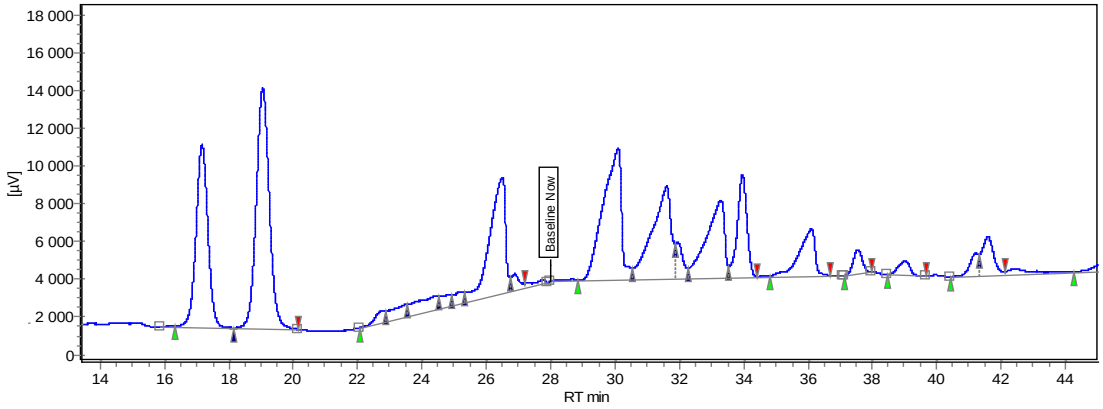
The difference with force baseline is that in this case, the markers of the first and the last peak are not modified.

Baseline now

This event forces the baseline to pass through the signal at the event time.



Becomes



This event is used to

- Bring the baseline back to the signal.
- Separate peaks which have a common baseline.
- End earlier a tailing peak.

The position of this event is relative to retention time drift, but as for most of the events, a similar peak-dependent event exists: “Baseline next valley”.

Baseline next valley

This event is similar to the previous one (Baseline now). The only difference is that CompassCDS waits for the valley following the event to bring back the baseline to the signal.

As a consequence, this event is best suited for separation of peaks having a common baseline, since “Baseline next valley” is less dependent on retention time variations from one analysis to another.

Shoulder Peaks:

To integrate a peak as the skimming of another, both peaks need first to be integrated. Thus it is important to define correct detection parameters (Set peak width and Set threshold) before defining the skimming parameters.

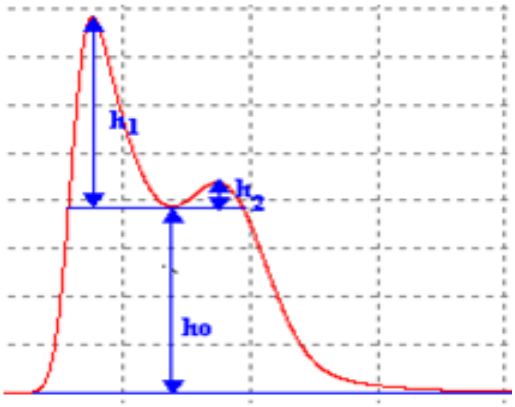
Set skim ratio

This event allows the user to set the shoulder integration threshold above a mother peak. This threshold must be associated to the events “Tangent skim front/rear” and “Exponential skim front/rear”.

A peak will be integrated as a shoulder peak on another peak, if its height satisfies the shoulder peak criterion.

In the following example, the second peak will be considered as a shoulder on the first peak if:

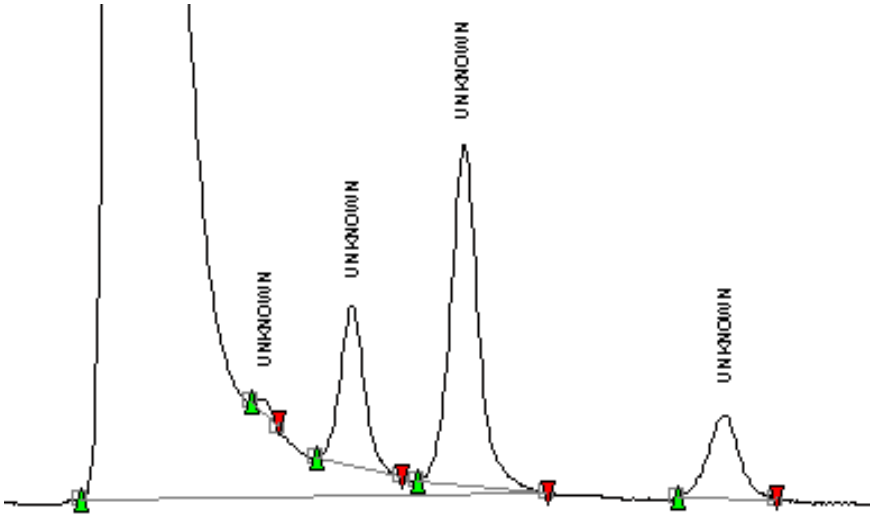
$$\frac{h_1}{h_2} \geq \text{parameter} \quad \text{and (ho} \neq 0)$$



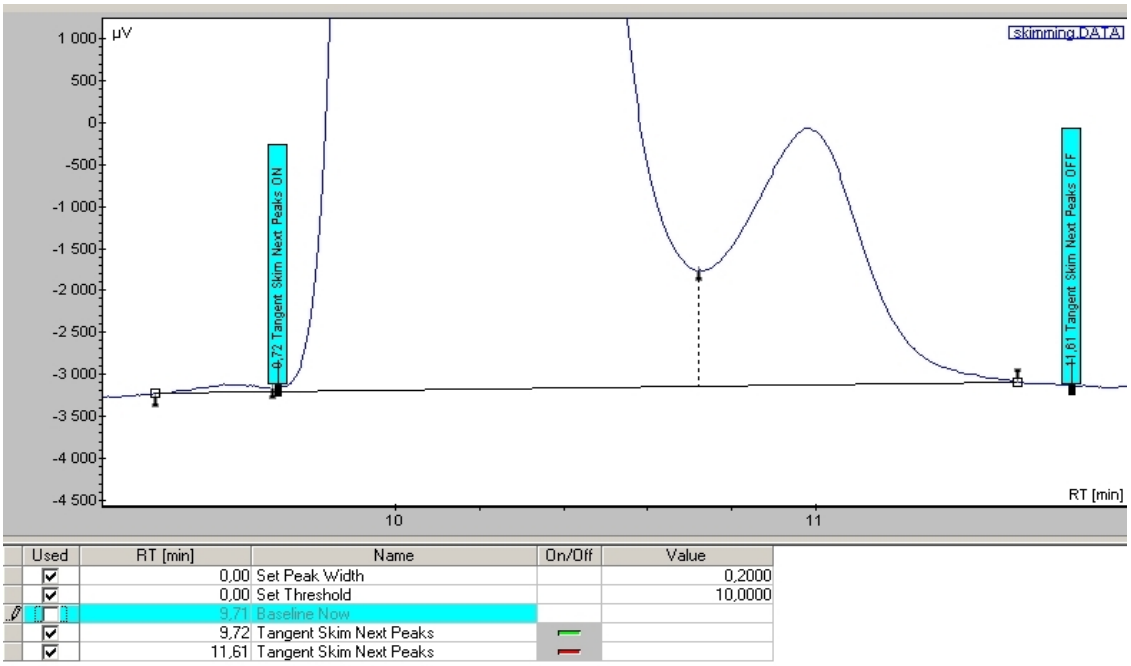
By default, this threshold is equal to 4.

Tangent skim next peaks On/Off

If this event is activated (On), all the peaks having a common baseline are integrated as shoulder peaks on the first peak, with a tangent baseline.

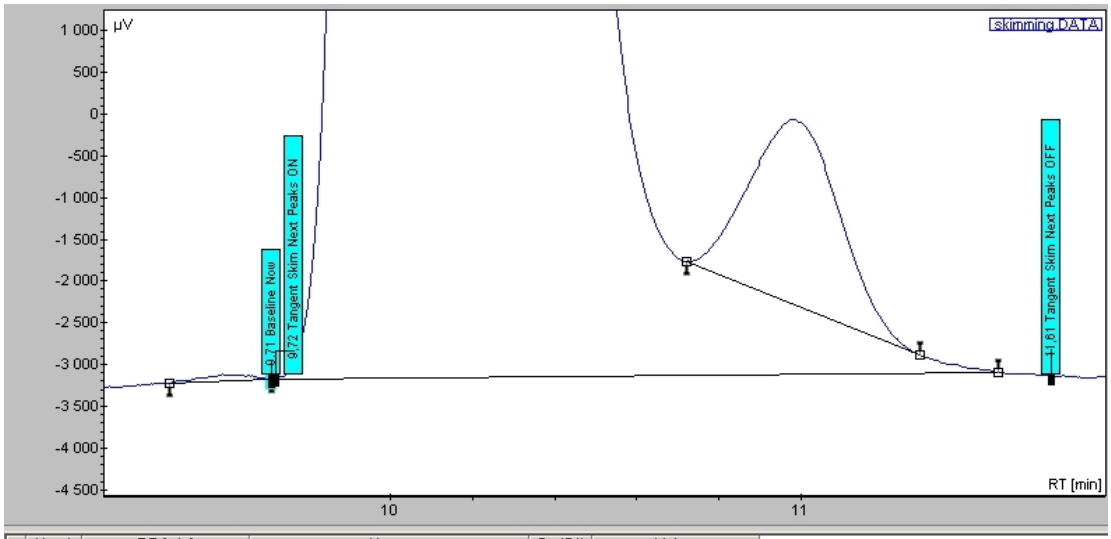


The tangent skim Next Peaks event does not work when the mother peak is not fully resolved (e.g., has a valley with the previous peak). The use of a Baseline Now event has the effect of removing the valley, and thus allows the skimming event to work properly. See figures below.



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,2000
☑	0,00	Set Threshold		10,0000
☐	9,71	Baseline Now		
☑	9,72	Tangent Skim Next Peaks		
☑	11,61	Tangent Skim Next Peaks		

Without the baseline now event, there is a group of three peaks sharing a common baseline



Used	RT [min]	Name	On/Off	Value
☑	0,00	Set Peak Width		0,2000
☑	0,00	Set Threshold		10,0000
☑	9,71	Baseline Now		
☑	9,72	Tangent Skim Next Peaks		
☑	11,61	Tangent Skim Next Peaks		

The baseline now event just breaks the group of peaks

Note that there is another event, more powerful, called Tangent Skim Rear, which handles such situations.

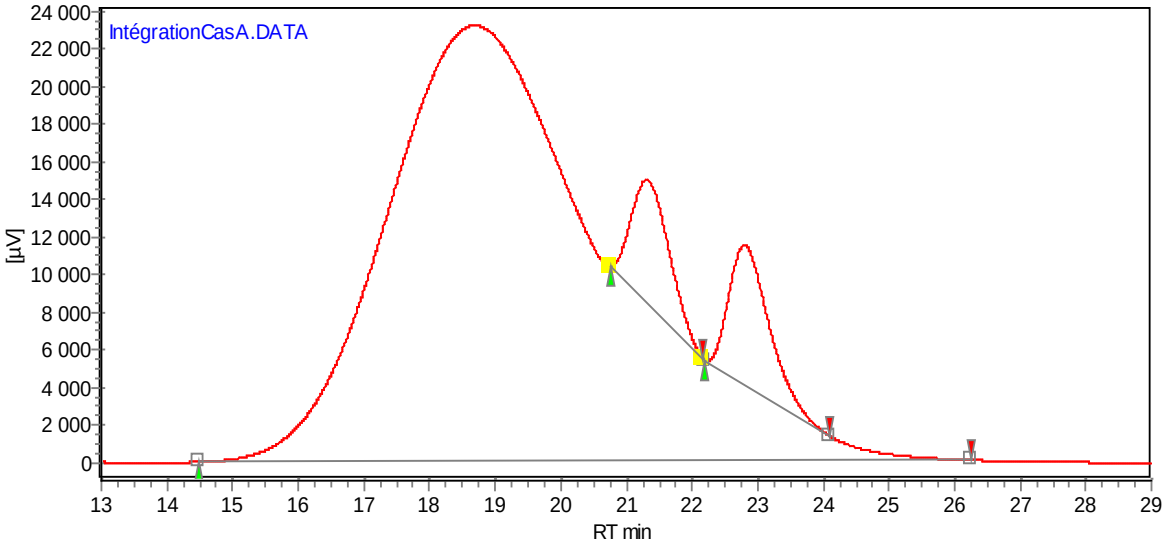
Exponential Skim Next Peaks On/Off

If this event is activated (On), all the peaks having a common baseline are integrated as shoulder peaks on the first peak, with an exponential baseline.

Tangent skims Rear/Front

Select this event to integrate one or several peaks as shoulders on a mother peak with a tangent baseline.

If CompassCDS detects poorly resolved peaks whose heights satisfy the above height criterion (see page 57), a tangent baseline is drawn underneath the shoulder peaks.

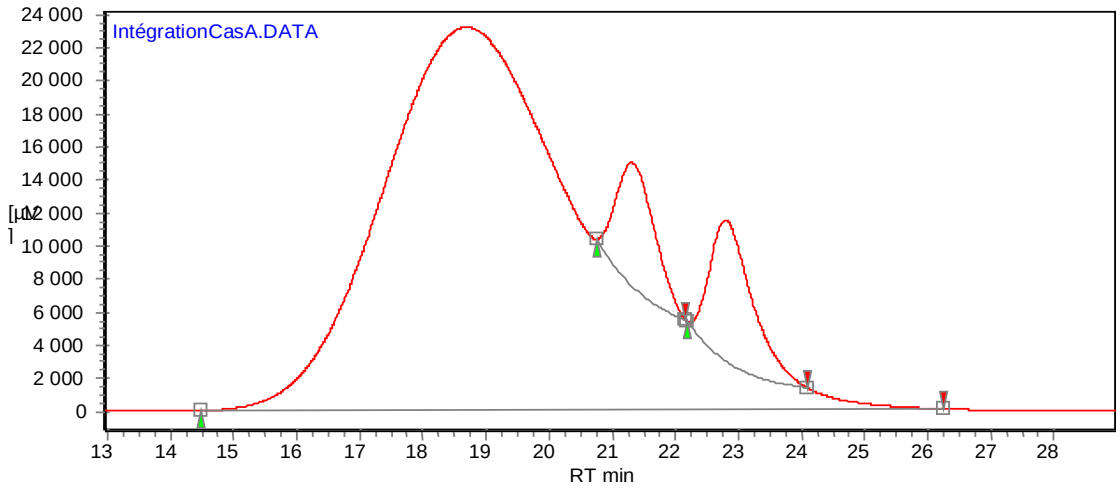


If the event is “Tangent skim front”, the shoulders are integrated before the mother peak. If the event is “Tangent skim rear”, the shoulders are integrated after the mother peak.

Exponential skim rear/front

Select this event to integrate one or several shoulder peaks with an exponential baseline.

If CompassCDS detects two poorly resolved peaks whose heights satisfy the above height criterion (see page 57), an exponential baseline is drawn underneath the shoulder peaks.



NOTE: The popup menu of the integration event table contains a Copy option that enables to copy the list of events before to paste it into another application.

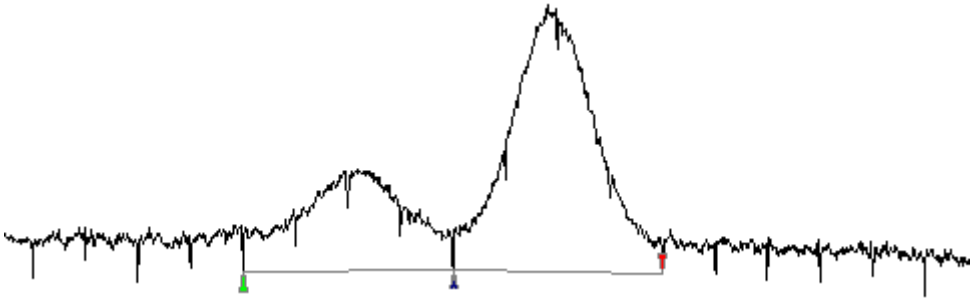
Integration Algorithm:

The integration algorithm operates in 4 stages: Spike reduction, data bunching, peak detection and baseline construction.

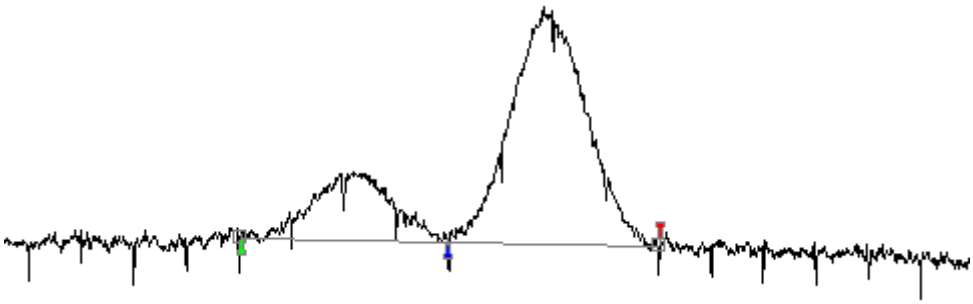
Spike Reduction

This stage is very useful if the signal is perturbed, and particularly with negative spikes. This stage can also be used to filter a part of the noise (and especially cyclic noise).

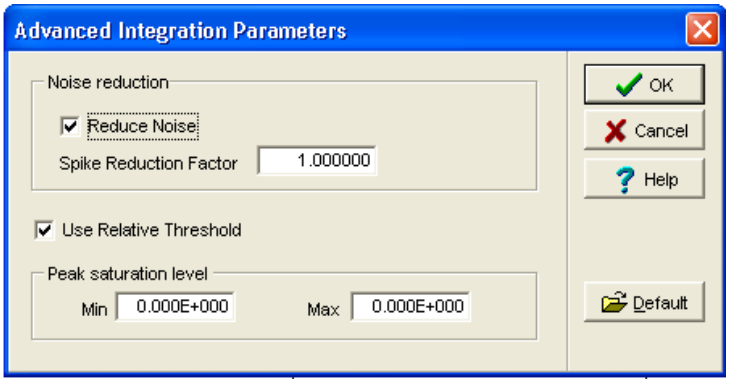
In the following example, some spikes perturb the chromatogram; the baseline is placed between the lowest points (the bottom of the spikes). Thus the area calculations are wrong:



If the spike reduction is activated, the spikes will be eliminated from the signal and the baseline drawn on this signal:



This step can of course be bypassed and the parameters defining the strength of the spike reduction can be modified. These parameters are defined in the advanced integration parameters, available using the METHOD / INTEGRATION / PARAMETERS menu:



Uncheck the Reduce noise box to deactivate the spike reduction.

Change the spike reduction factor to modify the way .is eliminated. The larger the spike reduction factor is the more noise will be eliminated. A value of Ø corresponds to no reduction. A value of 1 (default value) is generally a good compromise. In the above example, the specified value was 5. Be careful a too high value could eliminate small peaks.

Data Bunching

After the spike reduction, the chromatogram points are bunched and the peak starts and stops are detected. This step will eliminate some additional noise (random noise).

During data point bunching, the chromatogram is examined and every n point group is averaged into one point. Then the peak start and end determination is done with these bunched points.

Data bunching uses mean points in order to improve the peak start and end determination. The number of points that are bunched depends on the peak width defined in the integration method:

$$n = \frac{W}{15 \times \Delta t}$$

W is the peak width (in minutes) set in the integration method.

Δt is the acquisition period (inverse of the acquisition frequency), i.e., the time interval between two acquisition points (in minutes). This global variable is called DELTAT in the CompassCDS Chromatography Data System software.

A peak should contain at least 15 bunched points to be well detected.

Peak Start and End Determination

The peak starts and ends are determined using the bunched data points and the threshold entered in the integration method.

CompassCDS allows the integration of a chromatogram with two threshold types: normalized threshold (used by default) or absolute threshold.

Normalized Threshold

The threshold is “normalized” in order to reduce the influence of the injected amount:

$$Th_{norm} = Th \times \frac{Y_{max}}{100{,}000}$$

Th_{norm} is the normalized threshold

Th is the threshold entered in the integration method

Y_{max} is the maximum value of the signal along the chromatogram

Then, to determine peak starts and peak ends, the variation of the height between the bunched data is compared to the normalized threshold:

First of all, a peak start is searched:

If P1 is the height of a point, it is compared to P2, the height of the next point and P3, the height of the second next point:

Calling h1= P2-P1 and h2= P3-P2,

If h1> Th_{norm} and h2> Th_{norm} and if $\frac{h1+h2}{2}$ > Th_{norm} then a peak start is created in P1.

Then a peak apex is searched:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a peak apex is detected in P1.

After a peak apex, valleys or peak ends are searched:

Valley:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a valley is created in P1.

Note that the test is the same as for a peak apex, but after a peak apex if this test is positive, it means that there is a valley.

Peak end:

If P1 is the height of a point, it is compared to P2, the height of the previous point, P3, the height of the second previous point and P0 the height of the next point:

Calling h1= P2-P1, h2= P3-P2 and h3=P1-P0

If h1< Th_{norm} , h2< Th_{norm} and h3< Th_{norm} then a peak end is created in P1.

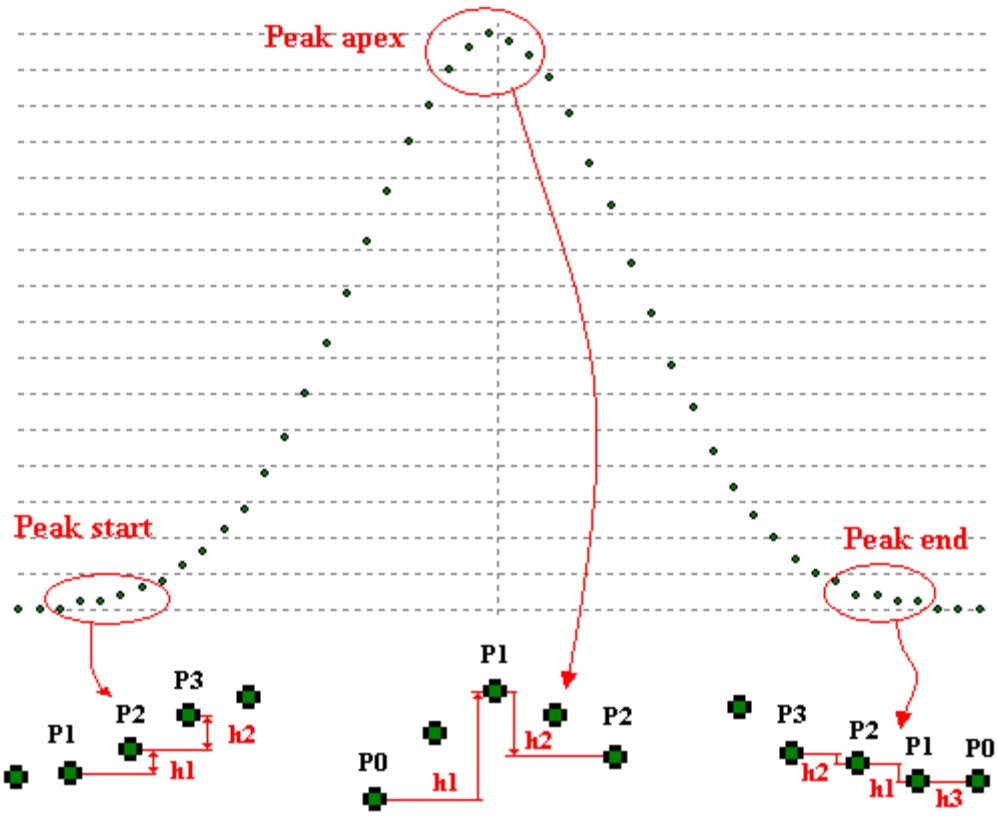
A peak apex is searched after a valley whereas a peak start is searched after a peak stop.

If negative peak detection is activated, the succession of peak starts, apexes, valleys and ends are the same, the test for peak apexes and valleys is the same as define above, the test for peak start and end is the opposite:

If h1<- Th_{norm} and h2<- Th_{norm} and if $\frac{h1+h2}{2}$ <- Th_{norm} then a peak start is created in P1.

If h1>- Th_{norm} , h2>- Th_{norm} and h3>- Th_{norm} then a peak end is created in P1.

Here are the ways the peak ends and apex are determined:

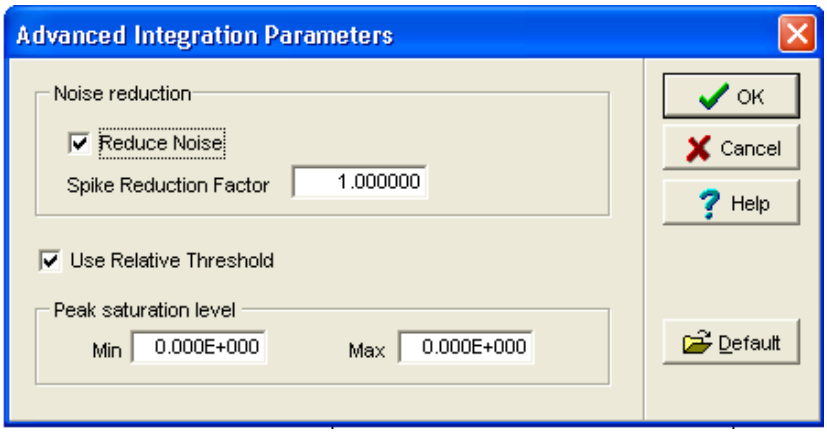


Afterwards the position of the marker is adjusted by considering only the points. The peak will be kept only if its area and height are larger than minimum values.

Absolute Threshold

In some analyses, the major peak size (solvent for example) changes a lot. If the normalization is made on the maximum height peak, this can modify the integration of the other peaks of the chromatogram. In these cases, it is advised to define an absolute threshold: select the METHOD / INTEGRATION / PARAMETERS menu.

The following screen is displayed:



Uncheck the Use relative threshold option.

Then CompassCDS defines the start and end of peaks.

First of all, a peak start is searched:

If P1 is the height of a point, it is compared to P2, the height of the next point and P3, the height of the second next point:

Calling h1= P2-P1 and h2= P3-P2,

If h1> Th and h2> Th and if $\frac{h1+h2}{2} > Th$ then a peak start is created in P1.

Then a peak apex is searched:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a peak apex is detected in P1.

After a peak apex, valleys or peak ends are searched:

Valley:

If P1 is the height of a point, it is compared to P0, the height of the second previous point and to P2, the height of the second next point:

Calling h1= P0-P1 and h2= P1-P2,

If h1×h2<0 then a valley is created in P1.

Note that the test is the same as for a peak apex, but after a peak apex if this test is positive, it means that there is a valley.

Peak end:

If P1 is the height of a point, it is compared to P2, the height of the previous point, P3, the height of the second previous point and P0 the height of the next point:

Calling h1= P2-P1, h2= P3-P2 and h3=P1-P0

If h1< Th , h2< Th and h3< Th then a peak end is created in P1.

A peak apex is searched after a valley whereas a peak start is searched after a peak stop.

If negative peak detection is activated, the succession of peak starts, apexes, valleys and ends are the same, the test for peak apexes and valleys is the same as define above, the test for peak start and end is the opposite:

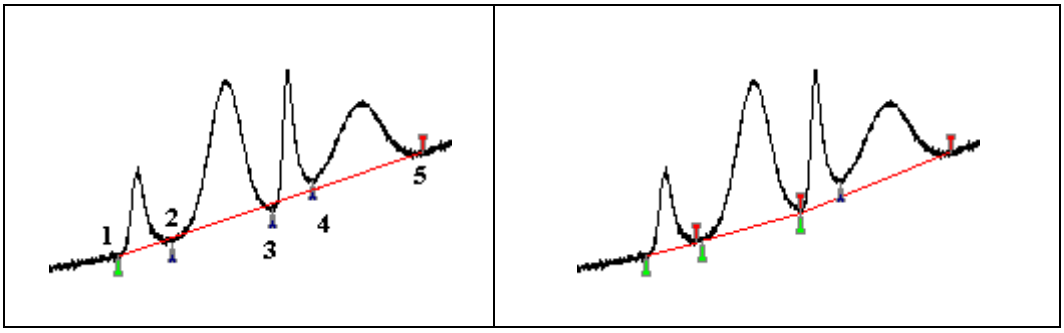
If h1<- Th and h2<- Th and if $\frac{h1+h2}{2} < -Th$ then a peak start is created in P1.

If h1>- Th , h2>- Th and h3>- Th then a peak end is created in P1.

Baseline Construction

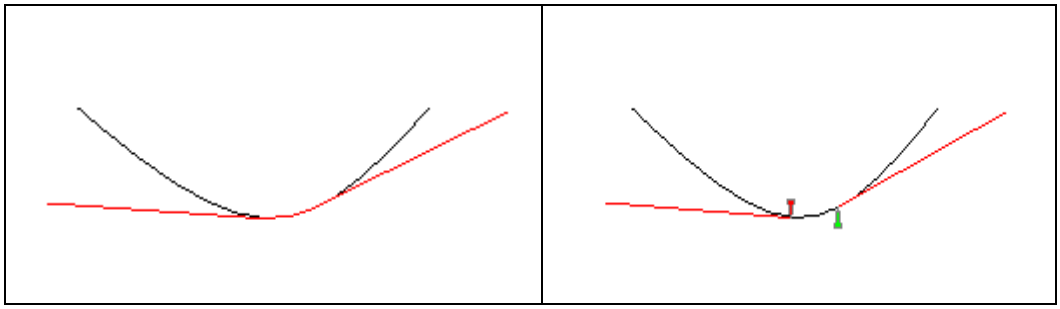
Where the peak starts and ends are defined, the baseline must be constructed:

A baseline is drawn between a peak start and the next peak end. The algorithm then checks that the baseline does not cross the chromatogram signal. If it does and negative peak detection is not activated, the baseline is modified by applying the tangent method in order not to intersect the signal.



Becomes

In the above example the baseline intersects the signal at points 2 and 3. Therefore the baseline is modified: it is drawn, as if it is a rubber band between the first peak start (1) and the last peak end (5). At points 2 and 3 the rubber band moves to follow the signal, e.g., when the baseline first touches the signal at 2 a peak end is generated and when it moves away from the signal, a new peak start is generated.



Peak Identification

This stage is used to identify peaks present in a chromatogram.

The Peak Identification Table

The first step is to fill out the identification table.

The identification table associates a peak, identified by its retention time to a name. It is possible to define reference peaks by checking the Reference peaks box. These are then used for the peak identification when differences in the retention times due to analytical conditions, occur.

How to build an identification table

To fill a table, press the right mouse button when in the table and a popup menu will appear.

Using the ADD menu option, insert as many lines as needed, then fill in the retention times and the names.

If the chromatogram has already been integrated, the identification table can be filled automatically with the retention times of all the peaks integrated in the chromatogram or peak(s) can be added one by one in the table.

First integrate the chromatogram by using either the icon, the F5 key, or by selecting the PROCESSING / INTEGRATE menu. Then,

- To list all the integrated peaks in the table, select the peak identification chromatogram method subsection and click within the peak identification page to access the popup menu, choose the INITIALIZE FROM CHROMATOGRAM option. CompassCDS will then paste the retention times and names for peaks (UNKNOWN-I) contained in the chromatogram (if any).
- To list only peaks of interest in the identification table, select the peaks one by one in the chromatogram picture, then select the Peak / Add to peak ID table option in the context menu. A line is automatically added in the peak identification table, the peak is temporarily named UNKNOWN-I, and its retention time is listed. The user will then be able to modify then name and the identification windows if needed.

Each line of the table represents one peak. In each line, enter the name of the compound corresponding to the peak, identified by its retention time and then choose the identification window width in the columns “Abs. Windows” and “Window percentages” and the identification mode.

It is also possible to fill the peak identification table from Excel. First define the peak names and RT in Excel (in columns and in this order), copy those parameters, and then select the ‘Initialize from clipboard’ option, available from the peak identification table context menu. The table is automatically filled The user can also copy an identification table, by using the ‘Copy’ option of the peak identification table context menu and paste it in Excel, then import the table in another method.

NOTE: Only the peak names and the retention times are imported from Excel in the identification table.

To delete an identification table line, highlight it by left clicking at the beginning of the line that is to be removed, then right click and choose DELETE CURRENT in the popup menu. To delete several lines, select them by left clicking in the first empty column of the table and drag the mouse to select several lines, and/or using the Ctrl and Shift keys as in any Windows application. Right click within the table to access the popup menu, then choose the DELETE SELECTION option. It is also possible to delete the entire identification table by choosing DELETE ALL in the popup menu.

The popup menu of the peak identification table contains a Copy option that enables its content to be copied and pasted into another application.

Identification table columns

Peak Name: The name of the compound corresponding to the peak. Two different peaks cannot have the same name.

Retention Time: The theoretical retention time of the peak. Two different peaks cannot have the same retention time.

Abs. Window: The absolute part of the identification window.

Window %: The relative part of the identification window.

These windows define the maximum interval around the retention time in which the peak will be assigned a specific compound name.

The absolute identification window is defined in minutes and in 1/100 of minutes. The relative identification window is defined as a percentage of retention time. If the relative identification

window percentage (Window %) is used, the larger the retention time is, then the wider the relative retention time window will be.

If retention time is RT, absolute window is Abs, and relative window is %W, a peak will be identified as the peak if its retention time is between

$$RT - Abs - \left(\frac{\%W \times RT}{100}\right) \text{ and}$$

$$RT + Abs + \left(\frac{\%W \times RT}{100}\right)$$

The identification window can thus be defined in minutes using absolute or relative windows, or defined using a combination of both.

The reference peak identification windows are treated separately. The reference peaks are identified first followed by all other peaks. If the reference peaks are correctly identified in these windows, it is possible to then define larger windows for reference peaks. This will ensure that they will be found, even if a retention time offset occurs.

NOTE: To display the identification windows, select the peak in the identification table and select the icon. If the retention time of the peak is recalculated according to reference peak(s), the window is centered on the recalculated time.

Cal.: This column selects which peaks are to be calibrated. There is a link between the identification and the calibration tables: each peak whose Cal. box is checked is added automatically in the calibration table.

Ref: This column appears only if the reference Mode is selected, which is indicated by the checked Reference peaks box.

To select reference peaks, check the Ref? box in the appropriate line(s) to indicate that the selected peak is now considered a reference peak. The theoretical retention times of the peaks will be corrected according to the difference between theoretical and experimental retention time of these peaks (see Non-reference peaks expected retention time).

The reference peaks must be chosen carefully. Reference peaks must be common constituents that will always appear in the chromatogram. If a reference peak is not present, another peak could be incorrectly assigned as the reference peak, and thus, the identification of the other peaks will be severely affected. Reference peaks should be easily recognizable. It is better to choose very high or large peaks or the last peak of the run (with the certainty that no other peak will occur afterward).

Mode: This column defines which peak will be chosen if several peaks are included in the identification window.

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the identification window.

Last: The peak will be the last peak found in the identification window.

Peaks are always listed in the retention time order.

Identification Process

Peaks are identified by their retention times, according to the identification window defined by user. In simple cases, peaks retention times are reproducible from one analysis to the other. In the case of non-reproducible retention times from one chromatogram to the other (due to analysis conditions, samples etc.), identification is more complicated and the definition of easily identifiable reference peaks is advisable. CompassCDS will identify in a first step the reference peaks and will estimate the time offset (according to the retention time) that will be applied during the identification of the other peaks of the chromatogram (non-reference).

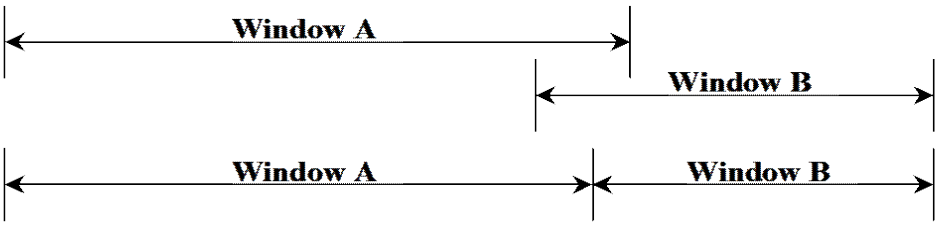
First, CompassCDS checks that the identification windows of the reference peaks do not overlap each other. If window overlap occurs, CompassCDS resolves the overlaps, and then the reference peak identification is processed.

Using the experimental reference retention times, CompassCDS calculates the other expected retention times, resolves the non-reference peak window overlaps, and the non-reference peaks are identified with these retention times and windows.

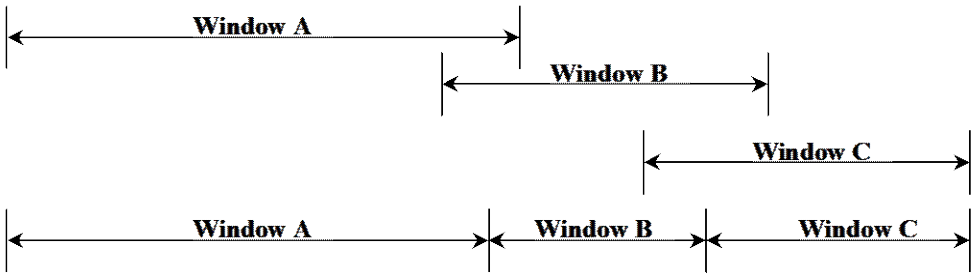
Since the reference and non-reference peaks are processed separately, it is possible to define larger reference windows because it does not matter if they overlap with the non-reference identification windows.

Resolving window overlap

If peaks are very close together, windows can overlap. This means that the end of an identification window can occur after the beginning of the next one. To cope with this problem, CompassCDS considers the common part of the windows, splits it in two, and assigns half to each window. For example:



If several successive windows overlap, the system resolves the first overlap (two first identification windows), then the next two ones. For example:



When using the relative identification windows (Window %), window overlaps can occur easily. If problems are encountered in peak identification, investigate what occurs during the window overlapping resolution.

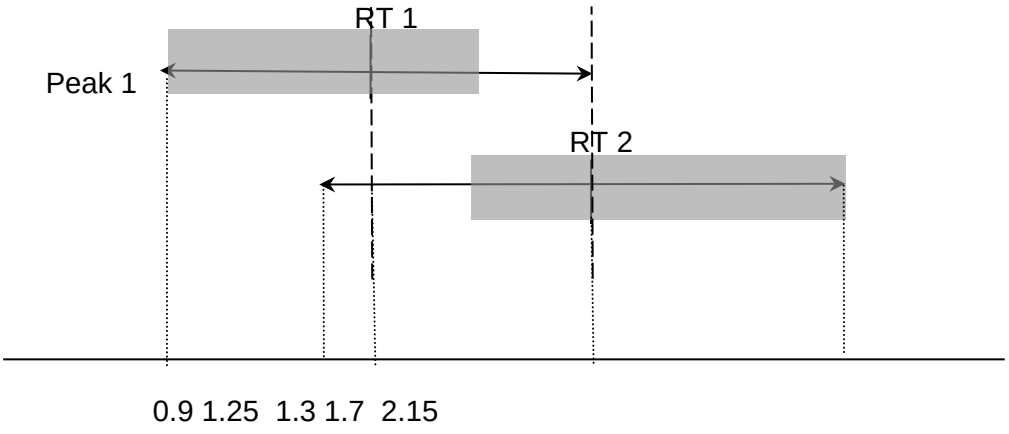
General Rule:

The window limit cannot go beyond the retention time of the previous or of the next peak. In this case the retention time of the previous/next peak is taken into account as the limit of the window, and the overlap is divided in two.

Example1: A peak retention time belongs to the identification window of another peak

Peak 1: RT1= 1.3 ID window: 0.4 min: [0.9 -1.7]

Peak 2: RT2= 1.7 ID window: 0.45 min [1.25 -2.15]



The identification window of Peak 1 becomes: [0.9-1.5] where 1.5 = RT1 + (RT2-RT1)/2

The identification window of Peak 2 becomes: [1.5-2.15] where 1.5 = RT2 - (RT2-RT1)/2

Example 2: a peak window belongs entirely to another.

Peak 1: RT1= 1.7 ID window: 0.45: [1.25 -2.15]

Peak 2: RT2= 1.99 ID window: 0.04 [1.95 -2.03]

The identification window of Peak 1 becomes: [1.25-1.97] where 1.97=RT1+ (RT2-RT1)/2

The identification window of Peak 2 becomes: [1.97 -2.03] where 1.97=RT2-(RT2-RT1)/2

Finding reference peaks

An identification window is defined for each peak.

A peak is identified as the reference peak if its retention time is found to be within the reference identification window. If there are no such peaks, the reference is not found.

If a reference identification window contains several peaks, the reference peak is chosen according to the selected reference window mode:

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the reference window.

Last: The peak will be the last peak found in the reference window.

Once the reference peaks are identified, CompassCDS will identify the other peaks.

Identification of the non reference peaks

Generally, the retention times are recalculated according to the two adjacent reference peaks. The formula for calculating the expected retention times for the non-reference peaks is:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_2 - RT_1}{RT_{ID2} - RT_{ID1}}$$

Where

RT is the expected retention time for a non reference peak.

RT1 is the real retention time of the reference peak preceding the peak.

RT2 is the real retention time of the reference peak following the peak.

RTID is the theoretical retention time of the peak defined in the identification table.

RTID1 is the theoretical retention time of the reference peak preceding the peak, defined in the identification table.

RTID2 is the theoretical retention time of the reference peak following the peak, defined in the identification table.

If peaks are eluted before the first reference peak: RT1 = RTID1 = 0. The index 2 is attributed to the next reference peak:

$$RT = RT_2 \frac{RT_{ID}}{RT_{ID2}}$$

If a peak appears after the last reference peak:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_1 - RT_0}{RT_{ID1} - RT_{ID0}}$$

Where RT0 and RT1 represent respectively the real retention times of the two reference peaks eluted before the peak of interest.

Note that this correction step works best when reference peaks are distributed throughout the entire chromatogram. In particular, be careful when using references that elute only at the beginning of a long run. They have a too strong impact on retention times at the end of the run. To minimize this effect, define a reference peak at the end of the run.

Once the system has calculated expected retention times for the remaining peaks, it centers the calculated identification windows on these times. If any windows overlap, the system will resolve the conflicts.

If several peaks fall within a window, the correct peak is chosen according to the selected identification mode:

Nearest: The peak will be the one whose retention time is the closest to the defined time.

Max height: The peak will be the highest one.

Max area: The peak will be the largest one.

First: The peak will be the first peak found in the identification window.

Last: The peak will be the last peak found in the identification window.

Note that if a reference peak is not found, its retention time will be the retention time set in the identification table, as if it had not shifted at all, therefore the identification of the peaks placed between the previous and the next reference peak may be affected.

If no reference peak is defined or found, peaks are identified by the retention times set in the identification table. Each peak retention time is compared to the identification window defined in the identification table.

Example:

For example, assume that three peaks exist in a chromatogram with theoretical retention times (saved in the identification table) of 5, 6, and 10 minutes.

When the sample is analyzed, the retention times have shifted to 6, 7.2, and 12 minutes. If the identification windows are 0.5 minutes wide, and reference peaks are not used, the peaks will not be identified.

However, if the last peak at 12 minutes is defined as the reference peak, and it elutes 1.2 times later than the defined theoretical retention time of 10 minutes, the expected retention times for the two other peaks (non-reference peaks) can be calculated.

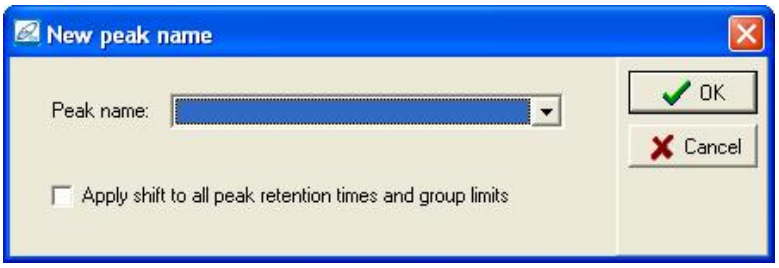
First peak: 5 x 1.2 = 6 minutes.

Second peak: 6 x 1.2 = 7.2 minutes.

The first two peaks can now be identified correctly with these new corrected retention times.

Peak re-identification

If a peak is bad identified by CompassCDS (due to a retention time shift for example), the user can re-identified it. Select the peak to re-identify in the chromatogram picture, then in the context menu, select the ‘Re-identification’ option. The following screen is displayed:



Select in the Peak name field, the name to assign to the selected peak. If you want that the software to apply the retention time shift to the rest of the peaks listed in the identification table, and to the group limits, select the ‘Apply shift to all peak retention times and group limits’ option. Note that the shift applied to the calculation of other peaks retention times or group limits is proportional to the time.

Group Identification

Result Groups and Calibration Groups

There are two types of groups: Result groups and Calibration groups.

- The result group adds the integration and quantification results of the compounds eluted in the time interval selected and /or the named peaks. The results are displayed in a table, displayed in the "results /group report" section of the chromatogram.
- The calibration group allows the user to quantify a group of peaks from a calibration curve or response factor. CompassCDS considers that all the integrated peaks present in the defined time period represent a single peak. A global calibration curve is built (or a global response factor entered in the calibration table) for the group. During this process, CompassCDS calculates a global quantity for the group (displayed in the group report), then sub-divides this quantity by peak according to its area percentage in the group and displays the individual results in the peak report: the ratio between peak quantity and the group quantity corresponds to the ratio between the peak area and the group area.

Do not forget to check the Cal. Box of each calibration group to be added in the calibration table. An interactive link exists between the peak and group identification tables and the calibration table.

The Group Identification Table

The group identification table contains four columns:

Group name	Group Type	Parameters	Cal.
GROUP1	Result group	0 range(s)	☐
GROUP2	Calibration group	0 range(s)	☐

Group Name: Specifies the name of the group.

Group type: Specifies whether the group is a result or a calibration group, which will induce the type of calculation that will be done for the group. It is possible to change it by accessing the list box.

Parameters: Defines the time limits (there can be several ranges) and/or names of the peaks to be added in the group.

Cal.: This column specifies the calibration groups to be quantified. A link exists between the group identification and the calibration table: each calibration group whose corresponding Cal. box checked is listed in the calibration table.

It is possible to either clear the entire table with the DELETE ALL popup menu (right click within the table) or delete single line as needed.

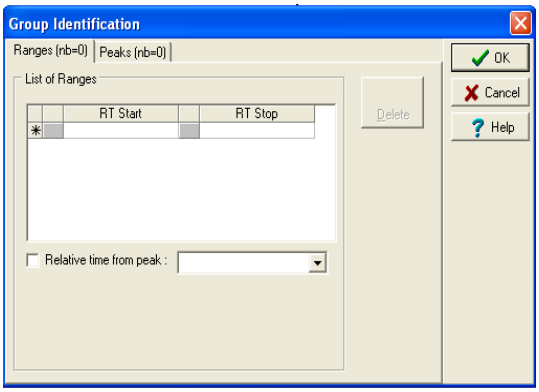
Identification of the Groups

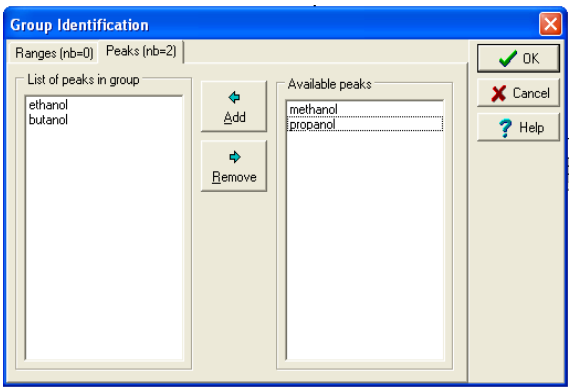
Peaks are added to a group based on their retention time or their name. It is possible to define a retention time interval or to select the name of the peaks to be added.

To add a group:

Click on Group identification in the browser.
Press the right mouse button in the group identification table.
In the popup menu, select ADD / RESULT GROUP or ADD / CALIBRATION GROUP.
Click in the Parameters column (left mouse button), and the Group identification dialog box appears.
In the Range page, enter the time limits of the intervals containing the peaks, or select them by dragging their name into the Peaks page.

- For the result group



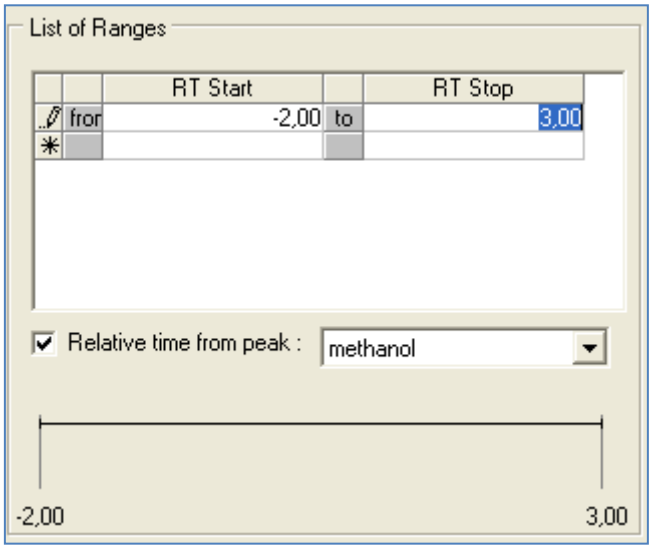


All results (area, height, quantity, etc.) of peaks belonging to the time range defined in the Range page and those named in the Peaks page are added.

NOTE: If 10 peaks are integrated within the time range of the group and only 3 are identified and quantified, then the group area will be the sum of the 10 peak areas. However, the group quantity will be the sum of the 3 peaks quantities (the quantity of the other 7 is considered to be equal to zero).

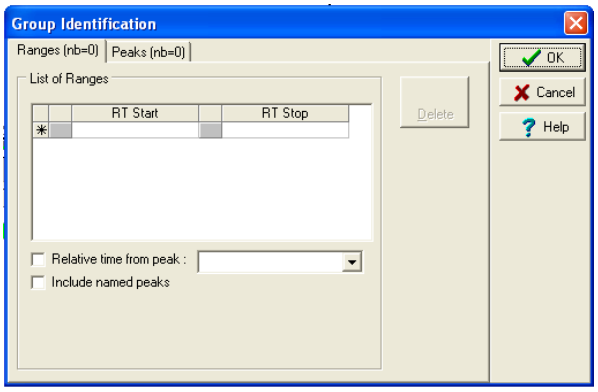
The time limits of a group can be defined relatively to a peak: In the Range screen, check the box ‘Relative time from peak’ and choose the name of a peak from the corresponding drop list: the

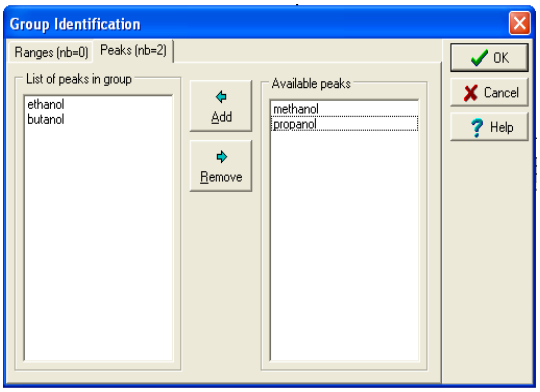
identification windows are defined based on the real retention time of this peak in the chromatogram. For example, to define a time range starting 2 minutes before the chosen peak and finishing 3 minutes after, define –2 and 3 in the time table and select the name of the peak in the ‘Relative time from peak’ scrolling list:



Several relative time intervals can be defined relatively to the same peak. To define those interval, select the peak name in the scrolling list and then define the interval times (take care to not overlay the intervals)

- For the calibration group:





By default the identified peaks whose retention times belong to the time range defining the group, are excluded from the group. To include them, select the option 'Include named peaks' or select their names in the page 'Peaks'.

The ‘Relative time from peak’ option has the same behavior than the one described in the result group section.

NOTE: In case a group is defined by a time interval: a peak is considered as a part of this group only if its apex belongs to the time interval defined. It is not necessary that both start time and stop time belong to the group time interval.

NOTE: In both cases, calibration group and result group, when reference peak(s) is (are) defined; the group interval time (based on a peak retention time) is calculated according to the recalculated peak retention time and not based on the theoretical one defined in the identification table. This allows correction of the shift of the retention times.

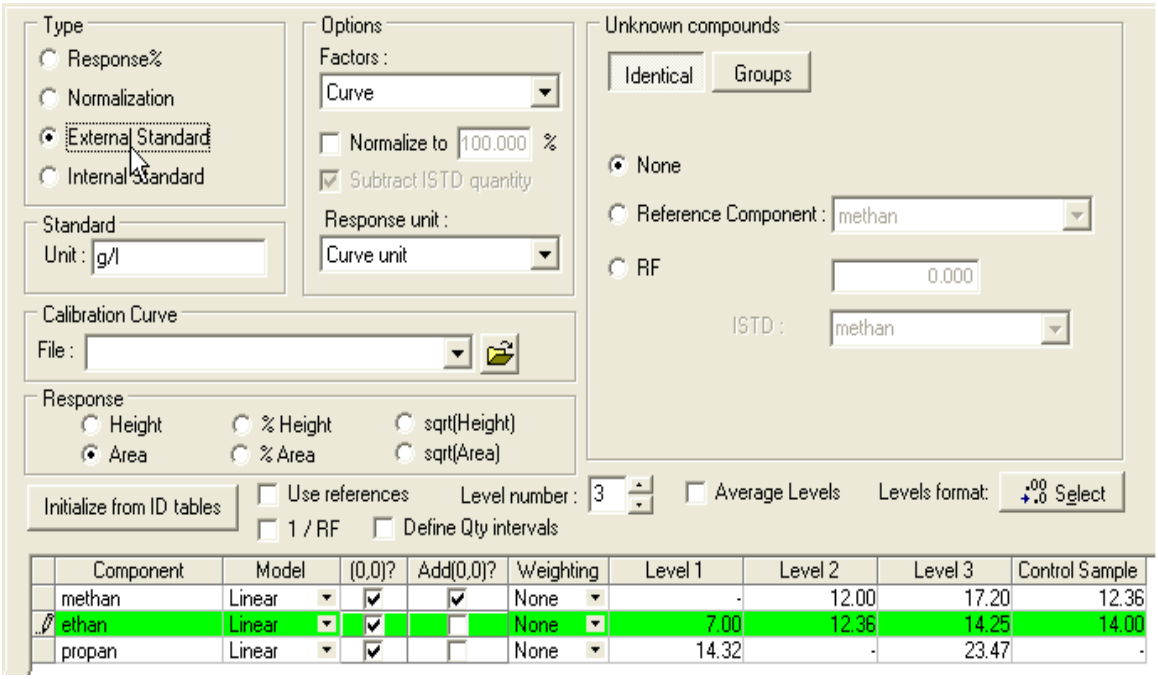
Quantification / Calibration

The aim of this step is to define the calibration parameters.

It is possible to work in two different calibration modes: Quantity versus Response or Response versus Quantity. The choice is made in the Configuration Manager.

Click on the calibration method in the browser to define the calibration parameters (or select the METHOD / PARAMETERS menu, or use the Ctrl+B key combination).

Now, define the different parameters for calibration: calibration type, response, factors, unknown compounds quantification, etc., proposed in the following screen.



Calibration Method Building

This part lists the steps to be followed in order to define a calibration method. Each step will be described in detail below.

In the Type section, select the calibration type. This selection determines how the quantification is calculated: Response %, Normalization, External Standard, or Internal standard. Details of these calibration types will be given in the paragraph "The Calibration Type" (see page 79).
To work with simple Response%, the calibration method is ready. For all other choices, additional parameters will need to be defined.
To work within the normalized mode (= external standard + normalization at a fixed percentage), check the Normalization option and enter the percentage value that the quantities will be normalized to in the 'Normalize to' field. By default, the results are normalized to 100 percent.
User can also check the External standard and the Normalize to cases, and enter the normalization percentage to obtain the same results.

It is also possible to normalize results in internal standard mode of calibration: check the 'Internal standard' and 'Normalize to' cases and enter the normalization percentage.
Define the response factor in the Factors field:

- Manual: If the response factor is known
- Curve: If the response factor is not known and that a calibration curve must be built
- Both: If some components have known response factors and others need the building of a calibration curve.

NOTE: If 'Curve' or 'Both' factor is selected, do not forget to enter a calibration curve name or select an existing calibration curve by pressing the button in the Calibration Curve section.

Specify the Response Unit in the corresponding field:

- Curve unit: Select Curve unit and precise this unit in the Standard Unit field (ppm, g/L, etc.)
- Mass%: To divide all the quantities by the sample mass (to display in the chromatogram properties) and multiply them by 100.
- Mass ratio: To divide all the quantities by the sample mass (to display in the chromatogram properties).

Note that in Normalization, only Curve unit is available.
In the Response section select the response mode. This selection determines how the peak will be processed- either by area, by height, by % area, % height, by area$^{1/2}$ or by height$^{1/2}$.
Configure the calibration table parameters:

- **Use references:** This option allows processing of one or several compounds listed in the table as another compound is defined in the table; which means with the same response factor or the same calibration curve. Enter in the 'Ref.' column the name of the reference peak.
- **1/RF:** This option allows user to enter inverse response factor.
- **Define Qty intervals:** This option allows user to define the interval in which CompassCDS must calculate the quantity of a compound, in the case of several solutions (polynomial models). Check the Use qty interval box for the concerned peaks, and enter the interval limits in 'Qty min' and 'Qty max' columns. If several solutions exist and this option is not selected, CompassCDS proposes the first strictly positive solution.
- **Level number:** to use for calibration building (curve or both factors). Enter the level number to use. The corresponding column number is displayed. The user has to complete those columns with the quantities associated to the level.
- **Average level:** When at least one calibration curve must be built, this option averages all the points of the same level before calculating the regression equation.
- **Levels format:** This option allows the user to modify the display format of the level entered in the table.

Calibration table filling: The content of the calibration table depends on the parameters selected: Calibration type, Response factor, Use reference, 1/RF, Define Qty intervals. The list of the columns that can be displayed is detailed underneath:

- **Component:** Lists the name of peaks and calibration groups to quantify in the table.

If the Cal. is checked for peaks and calibration groups in the peak and group identification parts in the method, they are automatically listed.

If all peaks and calibration groups (defined in the identification tables) must be listed in the calibration table, click onto the Initialize from ID tables' button. All the Cal cases will be automatically checked in the identification tables. An interactive link exists between identification tables and calibration table.

Note that peaks are listed in chronological order. Calibration groups are listed after the peaks, by definition order.

- **ISTD?** This column is displayed if the Internal Standard calibration type is selected. It allows entry of those components which are internal standards.
- **ISTD Name:** This column is displayed if the Internal Standard calibration type is selected. It allows association of an internal standard to each peak or calibration group.
- **Ref:** This column is displayed if the Use references option is selected. It allows definition of the peaks that will be used as reference for the quantification of other ones.
- **Model:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows the user to choose the mathematical model used for the calibration curve building
- **(0;0):** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'curve' or 'both'. It allows the user to force the curve pass through the point (0,0).
- **Add(0,0)?:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows the user to use the point (0,0) as a calibration point for the curve building. The curve will not necessarily pass through the origin, but the origin is taken into account for the calibration curve equation calculation.
- **Weighting:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is 'curve' or 'both'. It allows entry of a weighting of points during the calibration curve building.
- **Level-I:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is curve or both. It allows entry of the quantity of the compound for the calibration level I. If the compound is missing from the standard sample, enter '-' in the calibration table. No point will be added in the corresponding calibration curve for that level.

Response factor or 1/RF: This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'manual' or 'both'. It allows entry of the response factor for the compound or its inverse if the 1/RF option is selected.

- **Manual factor:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is 'both'. It allows entry of the components that will have a response factor.
- **Use Qty interval:** This column is displayed if the Define Qty intervals option is selected. It allows entry of the quantity calculation interval. This is useful when polynomial model is used, because several solutions can exist.
- **Qty min:** This column is displayed if the Define Qty intervals option is selected. It allows entry of the lower limit of the interval.
- **Qty max:** This column is displayed if the Define Qty intervals option is selected. It allows entry of upper limit of the interval.

This sets the way the unknown compounds (integrated peaks but not identified) are quantified. Two options are proposed: quantify all unknown compounds similarly by selecting the identical tab or according to retention time intervals by selecting the Groups tab.

Identical process for all unknown peaks:

- Choose none in the ‘Unknown compounds’ field to not quantify unknown peaks. The quantity of unknown peaks displayed in the result table is equal to 0.
- Choose Reference component to quantify unknown compounds by the same way as a peak present in the calibration table, and select the name of this peak in the scrolling list. If the calibration type is ‘Internal standard’, the internal standard associated is the one associated to the selected peak.
- Choose Response factor to quantify unknown compounds according to a response factor (RF or 1/RF whether the option 1/RF is selected or not) and enter the value of the response factor in the corresponding box. If the calibration type is ‘Internal standard’, select the name of the associated internal standard.

Unknown peaks are processed according to their retention time:

- Define the interval number in the ‘Groups’ tab, by activating the + and – buttons, and enter the start and the end of each group in minutes. Then enter for each group the way the peaks will be quantified (see previous paragraph).

The Response Mode

First, choose the response mode, to indicate whether the quantities are a function of the area, the height, the area %, the height %, area$^{1/2}$ or height$^{1/2}$ of the peaks.

By default, quantities are a function of the peak areas.

The Calibration Type

There are four options for calibration: response percentages, external standard, internal standard, and normalization. (The normalization type corresponds to normalization in external standard.)

Response Percentage

This is the simplest calibration mode, which is calculated based on the assumption that all integrated peaks have a response factor of 1, and therefore, the quantity associated with each peak corresponds to the ratio of its response (area, height, area%, height %, area$^{1/2}$ or height$^{1/2}$) over the sum of the response of all peaks.

The quantity Q of a compound is

$$Q = \frac{R}{\sum R} \times 100$$

Where

R is the response (area, height, area%, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

$\sum R$ is the sum of the responses of the chromatogram peaks

NOTE: When the results are normalized, the divisor and the multiplier factors cannot be used to modify the quantities.

NOTE: In response percentage mode, the results are always expressed in area% independently of the response mode: area, area%, area$^{1/2}$ (also, for height, height% or height$^{1/2}$, the results are always expressed in height %).

External Standard

Three response factor types are available: Manual, allowing user to manually enter the response factor of every peak to be quantified; Curve, allowing the building of calibration curves for all peaks; both, allowing the use of both curve and manual factors within the same method.

Manual Response Factors:

Choose ‘manual’ in the factors box.

In the case of manual response factors, the quantity Q of a compound is

$$Q = RF \times R \times \frac{M}{D}$$

Where

RF is the response factor of the compound read from the calibration table.

R is the response (area, height, area % height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

D is the divisor factor.

M is the multiplier factor.

Select ‘Curve unit’ in the response unit list box in order not to express the results in mass ratio or percentage, but in the same defined unit.

When the quantities are calculated, they can be manipulated as follows:

- They can be expressed in mass ratio relating to the sample mass:

The quantity Q of a compound becomes

$$Q = \frac{RF \times R}{m} \times \frac{M}{D}$$

where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

m is the mass of the sample (entered prior to acquisition, editable and modifiable in the chromatogram properties).

D is the divisor factor.

M is the multiplier factor.

To express the results in mass ratio, select Mass ratio in the Response unit list box.

- They can be expressed in Mass percentage relating to the sample mass:

The quantity Q of a compound becomes

$$Q = RF \times R \times \frac{100}{m} \times \frac{M}{D}$$

Where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

m is the mass of the sample (entered prior to acquisition and can be edited or modified in the chromatogram properties).

D is the divisor factor.

M is the multiplier.

To express the results in mass percentage, select 'Mass %' in the Response unit list box.

- They can be normalized to any strictly positive real number, up to 100. If this real number is Norm:

The quantity Q of a compound is

$$Q = \frac{RF \times R}{\sum (RF \times R)} \times Norm$$

Where

RF is the response factor of the compound.

R is the response (area, height, area %, height %, area$^{1/2}$ or height$^{1/2}$) of the peak.

Norm is the value of percentages normalization.

NOTE: As the results are normalized up to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

To obtain normalized results, check the Normalization box and enter the expected percentage.

NOTE: An alternative processing method is to choose the Normalization response type and then define the normalization percentage in the corresponding box.

NOTE: If the 1/RF option has been selected, the user enters the value of the inverse response factor in the calibration table and CompassCDS will calculate the value of the corresponding RF in order to apply the same calculations.

Curve Factors

Choose Curve in the 'Factors' box.

In case factors are read from a curve (Factors=curve), the calibration curve must first be built.

Calibration curve building:

When a calibration point is added to the curve, its coordinates are the response of the compound and the associated quantity.

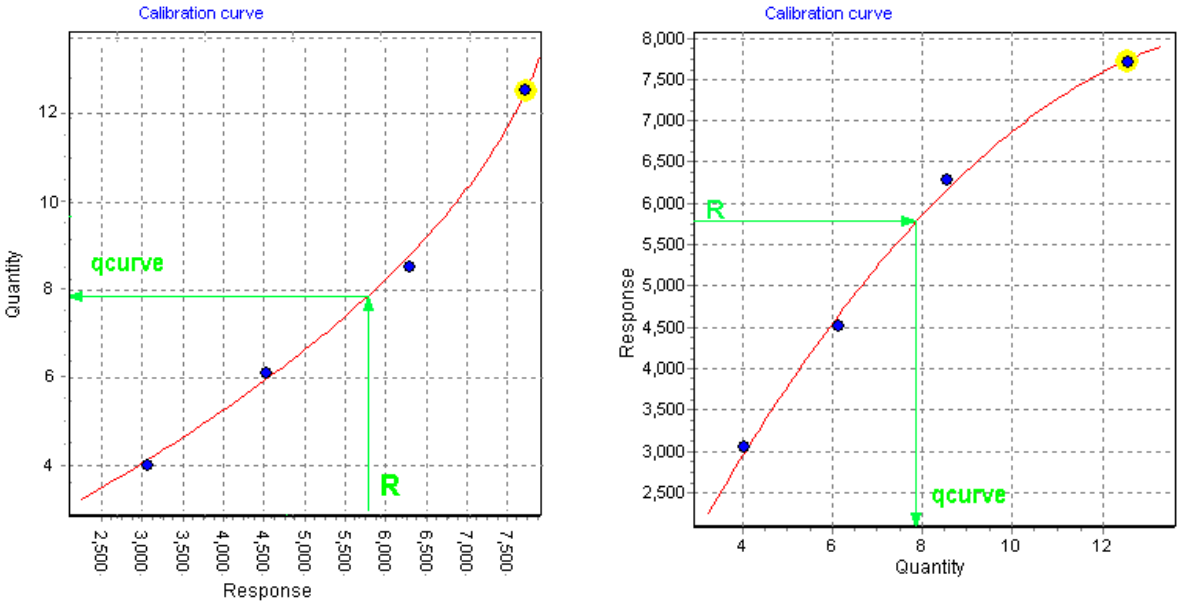
$q_{curve} = Q$ entered in the calibration table

NOTE: The multiplier and the divisor factor are not taken into account for the calibration curve building, except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

NOTE: If the response unit is 'Mass ratio' or 'Mass %', do not forget to enter a sample mass in the chromatogram properties, otherwise CompassCDS will not be able to build the calibration curve (even if the mass is not taken into account for the calibration curve building).

Quantification of unknown samples

The quantification of unknown samples is made using the calibration curve: a response corresponds to a quantity.



Quantity versus response orResponse versus quantity

The quantities read from the calibration curves are then corrected with M and D factors and turned into mass ratio or mass percentages:

If the Response unit is **Curve unit:**

$$Q = q_{curve} \times \frac{M}{D}$$

If the Response unit is **Mass ratio:**

$$Q = \frac{q_{curve}}{m} \times \frac{M}{D}$$

If the Response unit is **Mass percentage:**

$$Q = \frac{q_{curve}}{m} \times \frac{M}{D} \times 100$$

Results can also be **normalized:**

The quantity QNorm of a compound is:

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where Q is the quantity of the peak calculated in curve unit

$\sum Q$ is the sum of the quantities of the peaks

Both Factors

It is possible to work both with manual factors and calibration curves for the same chromatogram: Choose Both in the Factor zone. In the calibration table, the boxes in the column “Manual” must be checked for the compound whose factor is entered manually, then enter the manual factors in the corresponding column. For the other compounds, fill all the Level columns.

Note that the multiplier and the divisor factor are not taken into account for the standard calculation (Calibration curves building), except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

Internal Standard

The purpose of the internal standards is to compensate for the amount of injected sample when it can vary. If there are several internal standards, it is necessary to choose which internal standard is associated to each of the compounds.

As for external calibration mode, it is possible to use manual response factors, curve factors or both. Whichever process is selected, the user must still enter the quantity of the internal standard(s) for each chromatogram. These quantities can be entered:

- In the acquisition window for a Quick Start.
- In the 'Istd values' column for a sequence or a reprocessing list.
- In the chromatogram properties for a single reprocessing.

NOTES: When working in a curve factor unit, do not enter the internal standard quantity (ies) in the corresponding line of the calibration table; these values will be ignored.

In order to reprocess a chromatogram where the quantification method is different from internal standard (% response or external standard), using the reprocessing single functions (see page173), 2 steps must be performed:

First, reprocess the chromatogram as an unknown with the internal standard calibration method (in the 'method file' box). This step allows the user to define which compound(s) is/are internal standard(s).

Second, reprocess a second time the sample as an unknown or standard and enter the quantity of the internal standard(s) in the chromatogram properties.

Manual Response Factors:

Choose manual in the Factors box.

The response factors to enter are ‘Relative factors’, which means the response factor of the peak divided by the response factor of the associated internal standard. The response factor of the internal standard must thus be equal to 1.

In case of manual response factors, the quantity Q of a compound is

$$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Where

Qistd is the quantity of the associated internal standard, entered by user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier factor.

Select Curve unit in the response unit list box to express the results in user unit (g/L, ppm, etc.)

- Quantities can be expressed in mass ratio, relating to the sample mass:

The quantity Q of a compound becomes

$$Q = \frac{Q_{istd}}{m} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Where:

Qistd is the quantity of the associated internal standard, entered by the user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier factor.

m is the mass of the total sample including the internal standard mass(es) (entered prior to acquisition editable and modifiable in the chromatogram properties).

To express the results in mass ratio, select Mass ratio in the Response unit list box.

- Quantities can be expressed in mass percentage, relating to the sample mass:

The quantity Q of a compound becomes

$$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{100}{m} \times \frac{M}{D}$$

Where

Qistd is the quantity of the associated internal standard, entered by the user.

RF is the relative response factor of the compound.

R is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the peak.

Ristd is the response (area, height, area%, height%, area$^{1/2}$ or height$^{1/2}$) of the associated internal standard.

D is the divisor factor.

M is the multiplier.

m is the mass of the total sample including the internal standard mass(es) (entered prior to acquisition editable and modifiable in the chromatogram properties).

To express the results in mass percentage, select ‘Mass %’ in Response unit list box.

- Quantities can be normalized to any strictly positive real number, up to 100. If this real number is Norm:

$$Q' = \frac{Q}{\sum Q} \times Norm$$ Where $$Q = Q_{istd} \times RF \times \frac{R}{R_{istd}} \times \frac{M}{D}$$

Q is the quantity of the compound before normalization, and ΣQ is the sum of the quantities of the compounds before normalization. If the box Subtract istd mass is checked, the quantities of the internal standard(s) will be zero and will not be taken into account in ΣQ.

Note that as the results are normalized up to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

NOTE: If the option 1/RF has been selected, the user enters the value of the inverse response factor in the calibration table, CompassCDS calculates the value of the corresponding RF, and then applies the same calculations.

Curve factor

The relative response factors (response factor of the peak divided by the internal response factor) can be calculated from a calibration curve. For a compound or a calibration group, the quantity corresponding to the response is read from the calibration curve. This means that a calibration curve must first be built.

Calibration curve building

When a calibration point is added to a curve, its coordinates are the relative response of the compound and the relative associated quantity. The response is the response of the compound divided by the response of the internal standard. The relative quantity is the quantity entered for the compound in the calibration table divided by the internal standard quantity.

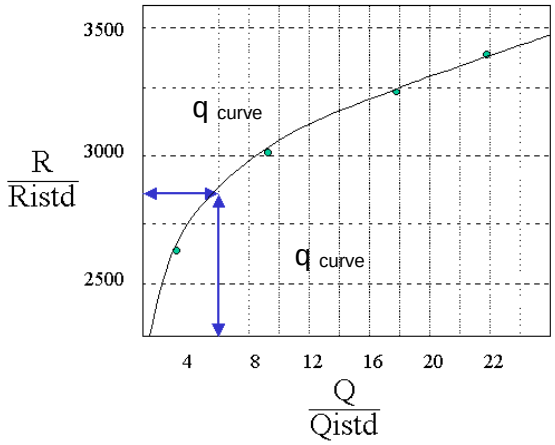
$$q_{curve} = \frac{Q}{Q_{istd}}$$

Q is the quantity of standard entered in the calibration table.

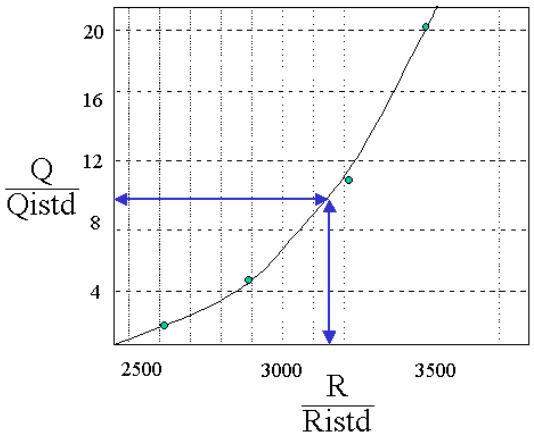
Qistd is the quantity of the internal standard entered in the acquisition window (Quick Start or sequence). Qistd can be modified in the chromatogram properties.

Note that the multiplier and divisor factors are not taken into account for the calibration curve building , except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

Quantification of unknown samples



Response versus quantity



Quantity versus response

For unknown samples, the calculation is the same as for the manual factor mode, except that the quantity ratios are read from the curve.

Those quantities are then corrected with the factors M and D and can be expressed as mass ratio or mass percentages:

If the Response unit is Curve unit:

$$Q = q_{curve} \times Q_{istd} \times \frac{M}{D}$$

If the Response unit is **Mass ratio:**

$$Q = \frac{q_{curve} \times Q_{istd}}{m} \times \frac{M}{D}$$

If the Response unit is **Mass percentage:**

$$Q = \frac{q_{curve} \times Q_{istd}}{m} \times \frac{M}{D} \times 100$$

Results can also be **normalized:**

The quantity QNorm of a compound is:

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where

$\sum Q$ Is the sum of the quantities of the peaks

For both mass ratio and mass% unit, m is the mass of the total sample including the internal standard mass (es) (entered before acquisition, editable and modifiable in the chromatogram properties).

Both Factors

It is possible to work with both manual factors and calibration curves for the same chromatogram: Choose Both in the Factor zone. The boxes in the column Manual must then be checked for the compound whose factor is entered manually in the calibration table.

Note that the multiplier and the divisor factor are not taken into account for the standard calculation (calibration curves building), except if the connected user owns the corresponding profile (to be defined in the CompassCDS Configuration Manager).

GENERAL NOTE FOR INTERNAL STANDARD CALIBRATION: It is possible to express the results after removing the internal standard quantities by checking the subtract ISTD mass option. This option is available with the three response unit proposed: curve unit, mass ratio and mass%. In the case of the response in curve units, the quantity of internal standards in the result table is equal to 0, and not included in the total quantity displayed.

In the case of the response in mass ratio or mass %, the quantity of the internal standard displayed in the result table is equal to 0, and for the calculation of the quantity of the other peaks, the mass taken into account is the mass entered by the user minus the sum of the quantities of the internal standard compounds.

The mass to enter is the sample mass after the addition of internal standard(s).

In the case of normalization, if Subtract ISTD mass is checked, the quantity of internal standard(s) is 0, and is not included in ΣQ.

Normalization

The normalization mode allows the user to calculate the ratio between each peak quantity, quantified using external calibration and the sum of all peak quantities, quantified using the same mode.

Note that the result is the same as the one obtained when selecting External calibration, checking normalization and defining a percentage in

.

The quantity QNorm of a compound is

$$Q_{Norm} = \frac{Q}{\sum Q} \times Norm$$

Where

Q is the quantity of the peak (calculated as described in the previous sections of the manual, according to the response mode: curve unit or manual factors)

$\sum Q$ Is the sum of the quantities of the chromatogram peaks

Norm is the value to which the percentages are normalized. By default, they are normalized to 100. Note that as the results are normalized to Norm, the divisor factor and the multiplier cannot be used to modify the quantities.

Response Factor Calculation: RF

The response factor is a variable calculated automatically by CompassCDS, equal to the quantity divided by the response. A response factor is calculated for each quantified peak or group, whatever the mathematical model defined in the case of 'Curve' factor.

The response factor of an unknown sample does not take into account:

- Multiplier factor
- Divisor factor
- Normalization factor
- Sample mass

CompassCDS proposes two variables 'RF' and 'recomputed RF', calculated as described in the following table:

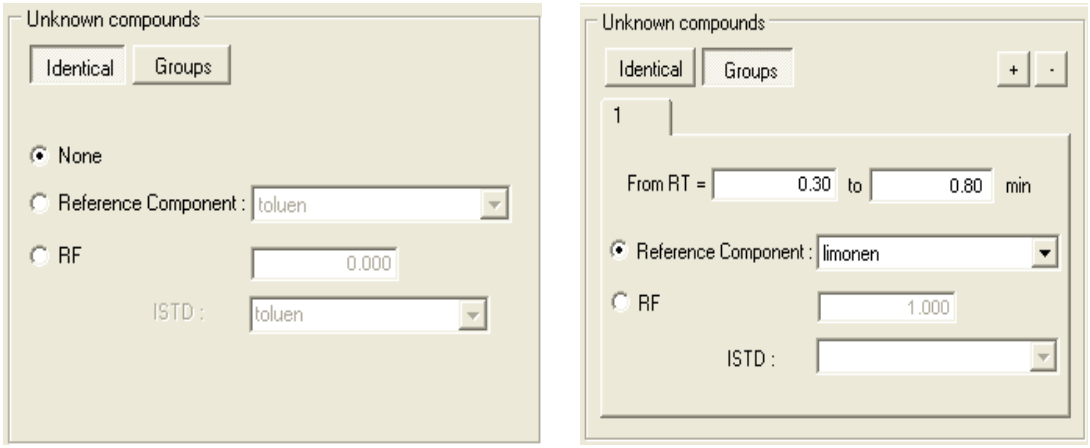
	CURVE factor		MANUAL factor	
Sample Type	RF	RF_Rec	RF	RF_Rec
Standard	$\frac{\text{Qty table}}{\text{Response}}$	$\frac{\text{Qty curve}}{\text{Response}}$	RF table	$\frac{\text{Qty}}{\text{Response}}$
Unknown	$\frac{\text{Qty curve}}{\text{Response}}$	$\frac{\text{Qty curve}}{\text{Response}}$	RF table	$\frac{\text{Qty}}{\text{Response}}$

Where Qty table is the quantity entered by the user in the calibration table, Qty curve is the quantity given by the calibration curve, and Qty is the quantity calculated by CompassCDS without taking into account the multiplier and divisor factors, the normalization factor and the sample mass.

In the case of internal standard, the calculated response factor is the relative response factor. It is equal to the ratio of the compound RF divided by the RF of its internal standard. The response factor of the internal standard is thus equal to 1.

A variable named RRF (reverse response factor 1/RF) can also be displayed in the result table.

Unknown Peak Processing



Unknown peaks (integrated but not identified) can be either all processed in the same way by using 'Identical' tab, or processed by groups defined according to time periods by using the 'Groups' tab.

Identical process for all unknown peaks:

It is possible to process unknown compounds in three different ways:

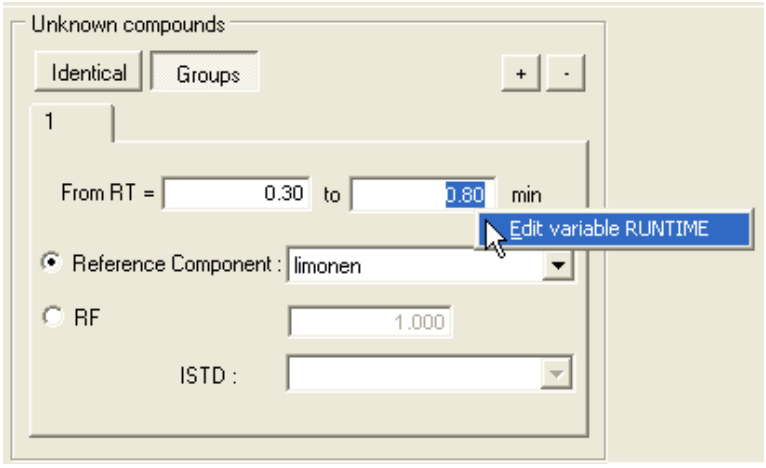
- **No processing:** Choose none in order not to quantify unknown compounds. A response factor of zero will be assigned for all unknown peaks.
- **Reference component:** In this case, the unknown samples will have the same response factor as the one specified in the list box. The reference peak is listed in the calibration table.
- **Response factor:** In this case, the unknown samples will have the response factor specified in the edit box, by default, this factor is one.

NOTE: If the calibration mode is internal standard, and if unknown peaks are processed with a response factor, it is necessary to choose the internal standard associated with unknown peak(s) in the internal standard box. Only one choice is available for all the unknown peaks.

Unknown peaks process according to retention time (groups):

It is possible to divide the chromatogram into time periods, and to process each period (group) differently. The group number is defined by activating + and – buttons. For each group, define the time period, and then choose the process to apply. The options proposed are the same as the 'Identical' tab ones.

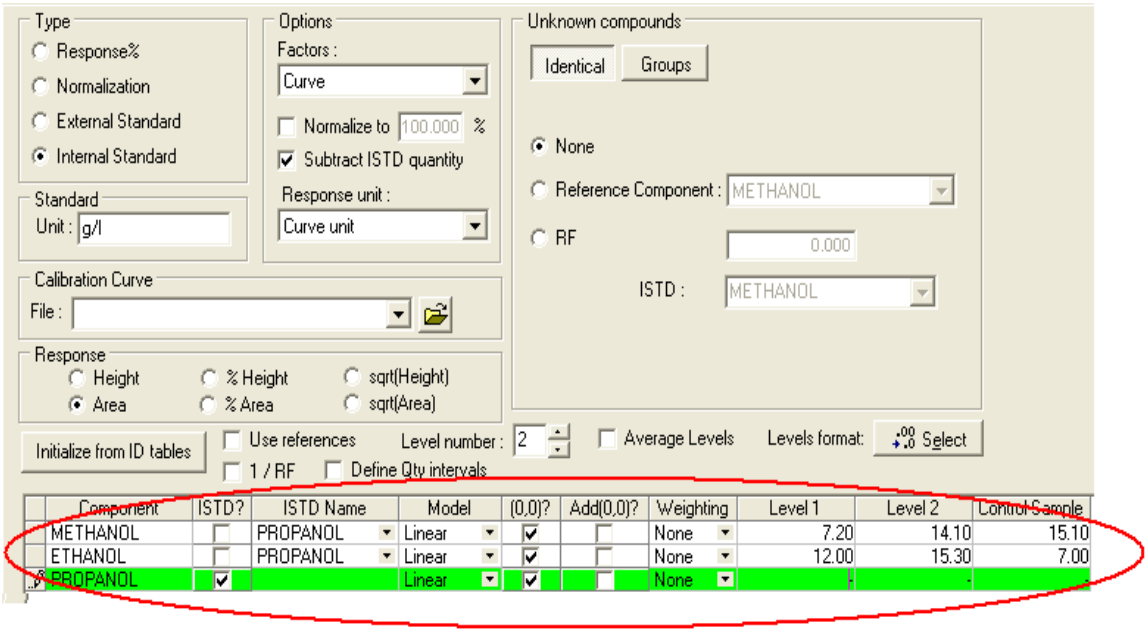
NOTE: It is possible to configure the format (number of significant digits, scientific format) of the group time limits and of the RF variable. Put the mouse cursor on the variable box that is to have its format changed, click on the right mouse button and select the 'Edit Variable XXX' option in the popup menu (XXX represents the variable name).



The variable screen is displayed and only allows the modification of the format for the selected variable.

The Calibration Table: As a Preliminary Step to a Calibration Curve Building

In the cases where the Curve and Both factors have been selected, the calibration table has to be completed.



If the user has checked the Cal. Boxes for peaks and calibration groups in the identification table, the names of these peaks and groups to be quantified are automatically imported into the calibration table. If a user wants all of the defined peaks and calibration groups to be imported into the

calibration table, without checking all the corresponding ‘Cal’ boxes, he must click on the ‘Initialize from ID table’s’ button.

A Control Sample column is displayed in the table. It allows the user to realize a suitability test on a control sample, by comparing the experimental quantity of the peak (in the control sample chromatogram) to the value defined in the table. Note that this value is theoretical and does not correspond to a calibration point.

Peaks are listed according to their retention time; calibration groups are displayed at the end of the list in their creation order.

A name must be defined in the Calibration Curve box, which is the name of the calibration file. This file will contain the curves for all the compounds defined in this table.

The number of calibration levels must be specified in the ‘Level number’ box, the corresponding column number will be displayed. The user must complete the table.

- **Model:** Several mathematical regression models are available:

Point to point: The calibration curve is composed of lines drawn between the calibration points.

Polynomial: It is possible to modify the order of the polynomial. A calibration curve can be modeled with up to a 5th order polynomial. The regression polynomial can be forced through zero (for example, in the case of a one-point calibration, the polynomial will be of order one and forced through zero).

If there are not enough points for calculation (e.g. only one point available for a 2nd order polynomial), the order of the polynomial is reduced and a message is displayed in the panel (below the polynomial coefficients).

Power: This is a $y= ax^b$ model.

Exponential: This is a $y=ae^{bx}$ model.

Logarithm: This is a $y=a + b \ln x$ model.

Average RF: Environmental laboratories in the USA routinely use a number of EPA approved methods and report formats for GC and GC/MS determination of analytes in matrices such as soil, air or water. Many of these methods require the use of the average response factor. To fit that need, CompassCDS provides a special model called Average RF.

If that model is chosen, it will imply automatically a linear model, force (0, 0) and 1/x2 weighting for the curve building. When the Averaged RF model is chosen, the other options which are set automatically cannot be changed until the calibration mode is changed.

- **(0; 0)?** Force the curve to go through (0;0).
- **Add (0, 0)?** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and the response factor is curve or both. It allows the user to use the point (0,0) as a calibration point for the curve building. The curve will not necessarily pass through the origin, but the origin is taken into account for the calibration curve equation calculation.
- **Weighting:** Different weighting models are available:

None: Gives the same importance to all calibration points.

x: This model calculates each calibration point using a weight proportional to the abscissa of the curve.

x^2: This model calculates each calibration point using a weight proportional to the square of the abscissa.

1/x: This model calculates each calibration point using a weight proportional to the inverse of the abscissa.

$1/x^2$: This model calculates each calibration point using a weight proportional to the square of the abscissa inverse.

log x: This model calculates each calibration point using a weight proportional to the decimal logarithm of the abscissa.

ln x: This model calculates each calibration using a weight proportional to the natural logarithm of the abscissa.

1-N: In this model, the weight of each new point is equal to the sum of previous point weights. For example, for 5 points, the weights are respectively: 1, 1, 2, 4, and 8.

- **Level-I:** This column is displayed if the calibration type is Normalization, External Standard or Internal Standard and that the response factor is curve or both. It allows entry of the quantity of the compound for the calibration level-I. If the compound is missing from the standard sample, enter '- 'in the calibration table. No point will be added in the corresponding calibration curve for that level.
- **Average levels:** If this option is checked, CompassCDS will average all calibration points of the same level (by compound) before building the calibration curve.
- **1/RF:** If this case is checked, the user has to enter the inverse of the RF (if manual response factor mode is used) in the corresponding column of the calibration table, and in the unknown compounds process field, if the unknowns are processed with manual response factor.
- **Use references:** A column 'Ref' appears. This option allows one or several compounds listed in the table to use the same calibration as another compound defined in the table that means with the same response factor or the same calibration curve. Enter in the 'Ref.' Column the name of the reference peak.
- **Define Qty intervals:** Three more columns are displayed, 'Use qty interval', 'Qty min' and 'Qty max'. This option allows user to define the interval in which CompassCDS must calculate the quantity of a compound, in the case of several solutions (polynomial models). Check the 'Use qty interval' box for the concerned peaks, and enter the interval limits in 'Qty min' and 'Qty max' columns. If several solutions exist and this option is not selected, CompassCDS uses the first strictly positive solution.

A Few Examples for Calibration

If you are not sure of how to configure the calibration method, please review the following examples which may be helpful.

1. External Standard with Calibration Curve building

To perform an external calibration, create a calibration curve for each compound of interest using standard samples. The amounts of each analyte in the standard samples for each level must be entered in the calibration table. These calibration curves are then used to determine the amount of each analyte in unknown samples.

The results for unknown samples are expressed in the same unit as the calibration samples.

How to proceed

- First, define the peak identification table.
- Then, in the calibration method: Choose External standard as the calibration type.
- Choose the response (Area, Height, Area %, Height %, and area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose Curve (since response factors are not yet known).
- In the calibration curve area, define the name of the curve to be built (or choose an already existing curve name using the open file box).
- Press the Initialize from ID table's button to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatically.
- Above the calibration table, enter the number of calibration levels to be used and then specify the quantities of the compounds for each level in the calibration table. Each calibration level corresponds to a calibration standard.

The calibration method is ready.

Calculation of relative response factor

To specify response factors relative to a reference compound, a user must create variables. Two cases are treated according to the reference compound remains the same or not.

How to proceed

Fixed reference compound: For example, if this reference compound name is 'Benzene', a variable called 'Relative RF' must be created, which would be a peak variable with the following formula: 'RF/RF('Benzene')', then the relative response factors can be displayed in the peak result table.

Variable reference compound: Two variables must be created. The first one could be called 'Ref Name', which would be a global and user input variable. The second one could be called 'Relative RF', which would be a peak variable with the following formula: 'RF/RF(Ref Name)'. A default value (name of the reference compound) can be specified in the acquisition method and the reference compound can be changed before each run in the acquisition window. The relative response factors can then be displayed in the peak result table.

Normalization to a Value

The sum of the compounds present in the sample to analyze represents a well-known percentage of the mother solution (50% for example). The response factors of peaks to quantify are known.

The results should be expressed in quantity percentages.

How to proceed

- First, specify the peak identification table.
- Then in the calibration method: Choose Normalization as the calibration type.
- Choose the response (Area, Height, Area %, Height %, area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose 'Manual'.
- In the next edit box (Normalize to) enter the value to which the results should be normalized: 50.
- Press the 'Initialize from peak ID table' button to import all the identified peaks, or check the 'Cal'. Box of each peak of interest in the identification table to make the import automatically.
- In the calibration table, specify the response factors for each of the peaks and calibration groups.

The calibration method is ready.

NOTE: If you want to quantify unknown compounds and give them a response factor of 1, select in the ‘unknown compounds zone response factor’ and enter 1.

Internal Standard, Result in Mass %.

Build a method to analyze sample owning defined peaks and groups in internal standard calibration type. The user knows the relative RF of each peak and calibration group. Unknown peaks are processed with the RF of an identified peak.

The results should be expressed in percentages of total sample weight.

How to proceed

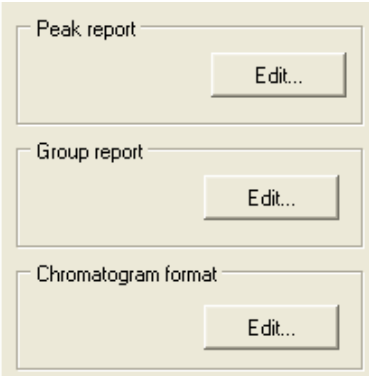
- First, specify the peak and group identification tables, take care to specify Calibration groups for the groups containing only the peaks that must be quantified with the same response factor.
- In the calibration method: Choose Internal standard as the calibration type.
- Choose the response (Area, Height, Area %, Height %, and area$^{1/2}$ or height$^{1/2}$) to be used.
- In the Factors area, choose Manual.
- In the Response unit zone, choose Mass % (since the responses are to be divided by sample mass and multiplied by 100).
- In the Unknown compounds zone, select the identical tab, check ‘Reference component’ and choose the name of the reference component.
- Press the ‘Initialize from ID table’ button to import all the identified peaks, or check the ‘Cal.’ box of each peak of interest in the identification table to make the import automatically.
- In the calibration table, specify the internal standard and the response factors of each peak and calibration group.

The calibration method is ready.

If the internal standard quantity is strictly the same for standards and unknowns, you should enter this quantity in the method acquisition part before chromatogram acquisition. It will be possible to modify this value in the Quick Start window or in the sequence.

Formats

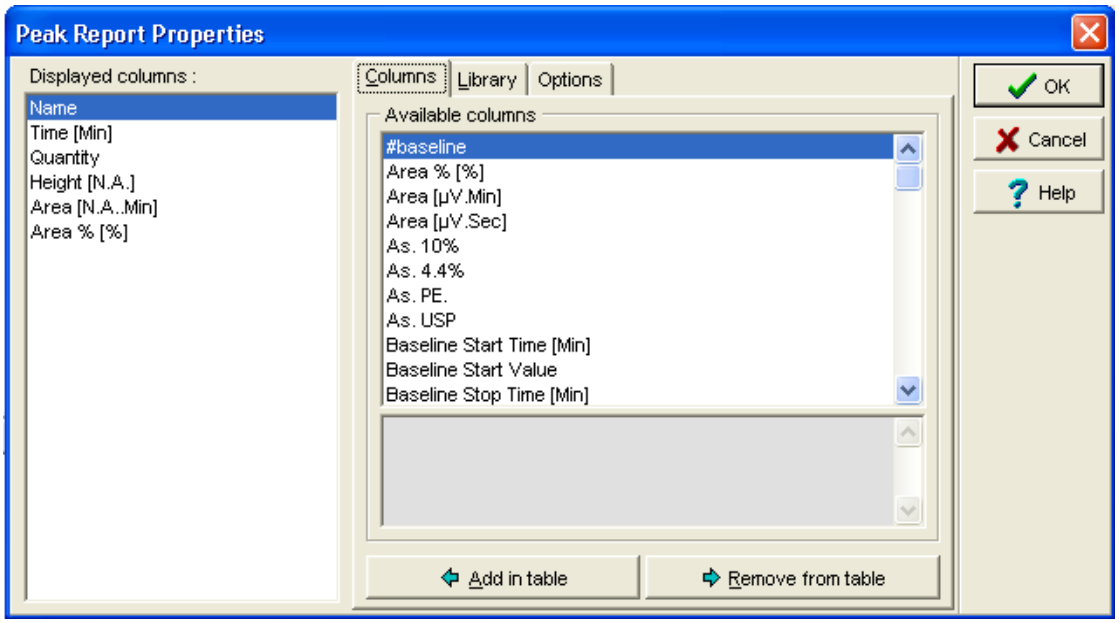
This section is accessible from the method or using the shortcut Ctrl+F, allows configuration of chromatogram, peak table and groups table formats.



The Peak Table Format

The purpose of the option is to configure the columns to display in the peak results table. Click on the Edit button in the ‘Peak report’ part.

The following screen is displayed:



NOTE: This screen is also accessible from the result peak table. Click on the right mouse button in the table, and choose REPORT PROPERTIES in the popup menu. The peak report properties appear.

This screen is composed of three sections:

Displayed columns: In this section, the variables to be displayed in the result table are listed in the right order.

Available columns: In this section, the variables calculated by CompassCDS are displayed. In order to make the software calculate another variable, define the variable in the variable editor (peak variable), and then it will appear in the available columns.

The gray section placed under the ‘Available column’ zone displays a description of the variable selected in the ‘Available column’ zone.

To add or remove a column from the report: Either click and drag the variables from the ‘Available column’ zone to the ‘Displayed column’ zone or from the ‘Displayed column’ zone to the ‘Available columns’ zone or select them with the mouse and click on the buttons

and

, or double-click on the name of the variable to add in the 'Available columns' or on the name of the variable to remove from the table in the 'Displayed columns'.

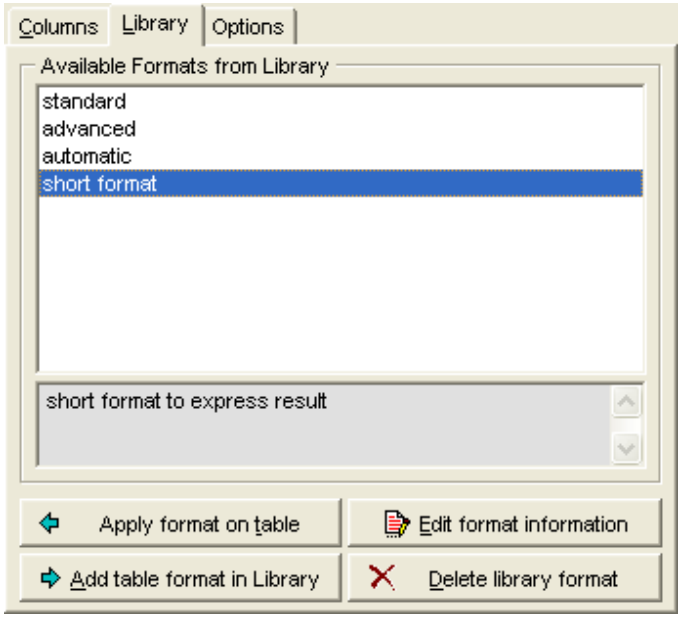
To change the report column order: In the ‘Displayed column’ zone, click and drag the variable to modify their order in the table:

The options page:

- **Show unknown peaks:** By default unknown peaks are shown in the peak table. But when this box is unchecked, only the identified peaks are displayed. When no peak is displayed in the peak report, it indicates that no peak is identified and this box is checked.
- **Display index column:** A column corresponding to the peak indices is displayed in the peak report. It is possible to hide this column by unchecking this box.
- **Show missing peaks:** The missing peaks (not identified in the chromatogram) are listed in the result table with their theoretical RT. The ND (not defined) value is assigned to other variables.

The Library page

It can be of interest to save a format as template, to apply it in several method, or printed report, or expected files. To do that, select the library tab, the following screen is displayed:



Click on the

button. A window appears, in which the name of the format can be saved with an entry field to provide a short description of the format.

The format is then added to the available formats. By clicking on the format, the description of the format is displayed in the gray zone.

In a different method, click on Apply format on table, and the peak report format is displayed in the 'Displayed column' zone.

To delete an obsolete format, select the format and click on Delete library format.

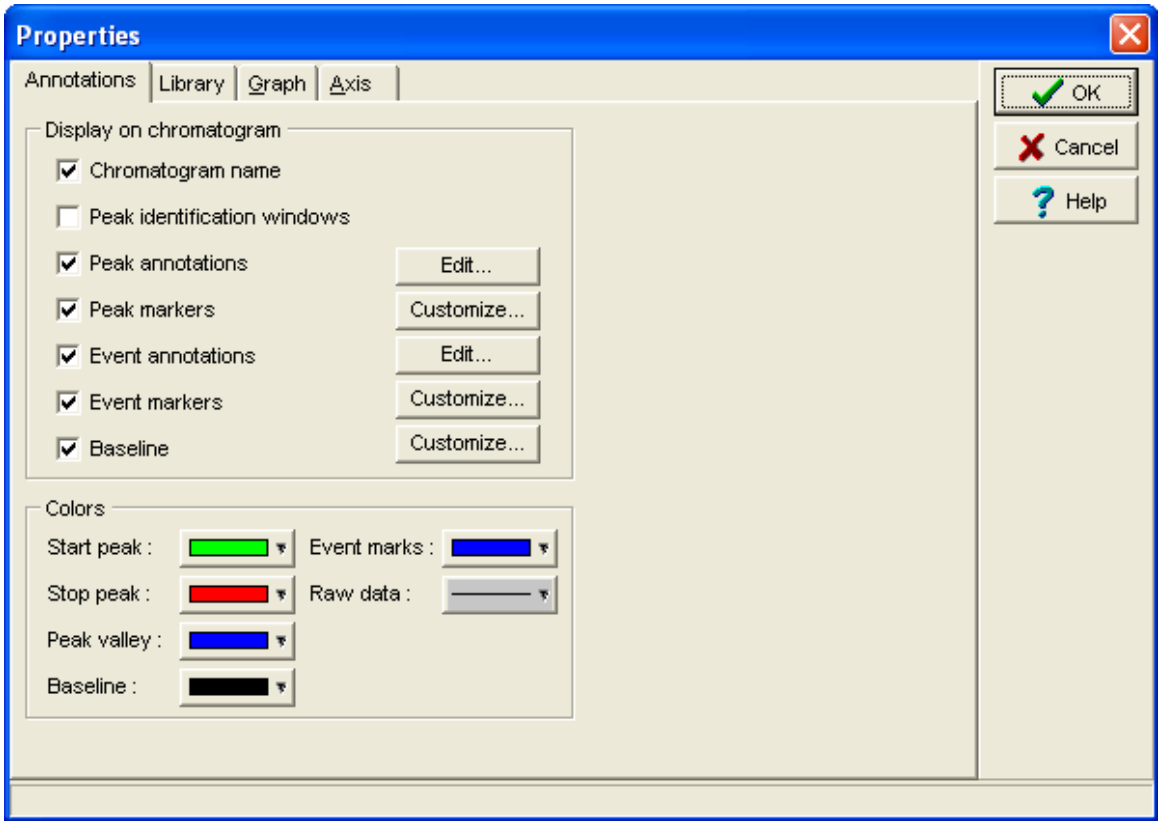
To change the name or the description of a format, select the format and click on Edit format information.

The Group Table Format

The group table can be customized as the peak table, e.g., in the report properties it is possible to change the displayed variables and to create formats. These formats will be accessible from CompassCDS Report Editor and in other methods or chromatograms. It is also possible to save group formats in a library.

The Chromatogram Format

Click on the Edit button in the "Chromatogram format". The following screen is displayed:



Four tabs are proposed: Annotations, Library, Graph, and Axis.

Annotations

- Check or Uncheck Chromatogram name to display or not the name of the chromatogram onto the chromatogram chart. This can be useful to copy/paste the chromatogram picture from CompassCDS to another application (Word, Paint, etc.) without the chromatogram name. This option is also applied when printing a chromatogram from the Workspace option (see corresponding chapter).

NOTE: If saving a library without the ‘Chromatogram name’ option, and use this format in the report style/ Chromatogram object, the name of the chromatogram will nevertheless be printed on the chromatogram picture.

- Check Peak identification windows to display the identification windows on-screen (Corresponds to pressing the icon). The peak identification windows are shown only one after the other when the identification method is displayed: The identification window will be displayed when the corresponding line is selected in the peak identification table.
- Check Peak annotations to display the peak annotations that contain information for every peak on the chromatogram (Corresponds to pressing the icon). Press the Edit button (or the icon in the toolbar) in the Peak annotation screen to change the annotation content.
- Check Peak markers to display the markers that symbolize peak start and end (corresponds to pressing the icon . The colors of these markers can be modified (see below). Press the Customize button to change the peak markers style (cross, rectangle, triangle, circle.) and the size.
- Check Event annotations to display the integration events on the chromatogram at the time they are defined (Corresponds to pressing the icon). Press the Edit button (or the icon in the toolbar) to change their appearance in the Event annotations screen (see page 186).
- Check Event markers to display markers on the chromatogram at the times the integration events are defined (corresponds to pressing the icon). Press the Customize button to change the event markers style (cross, rectangle, triangle, circle) and the size.
- Check Baseline to display the baseline joining a Start and an End peak marker (corresponds to pressing the icon). Press the Customize button to change the baseline markers style (cross, rectangle, triangle, circle.) and the size.

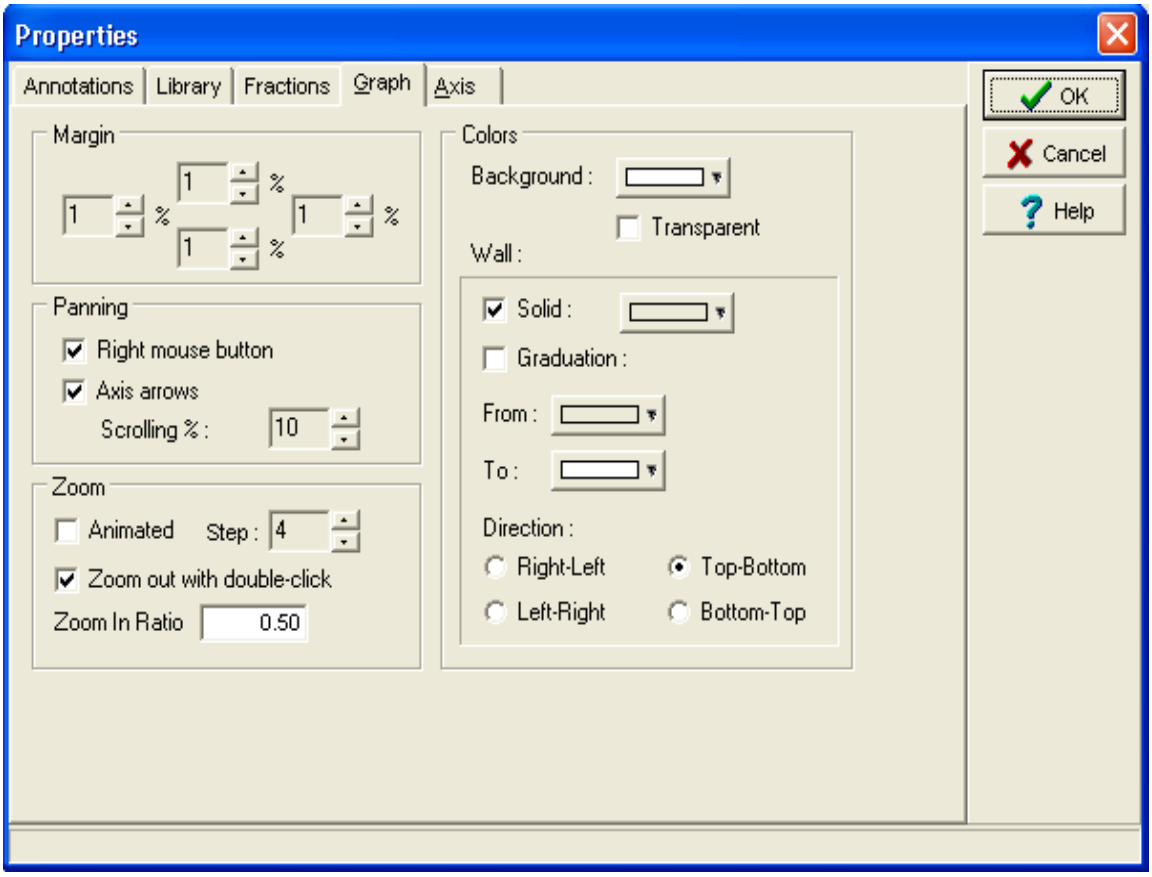
The colors of these markers can also be changed in this screen: start peak, stop peak, peak valley and event markers, including the baseline color.

The raw data color, the corresponding size and thickness of the plot can also be customized.

NOTE: The same screen is displayed from the chromatogram: Press the right mouse button within the chromatogram and select PROPERTIES in the popup menu or press the Chromatogram annotations icon .

Graph

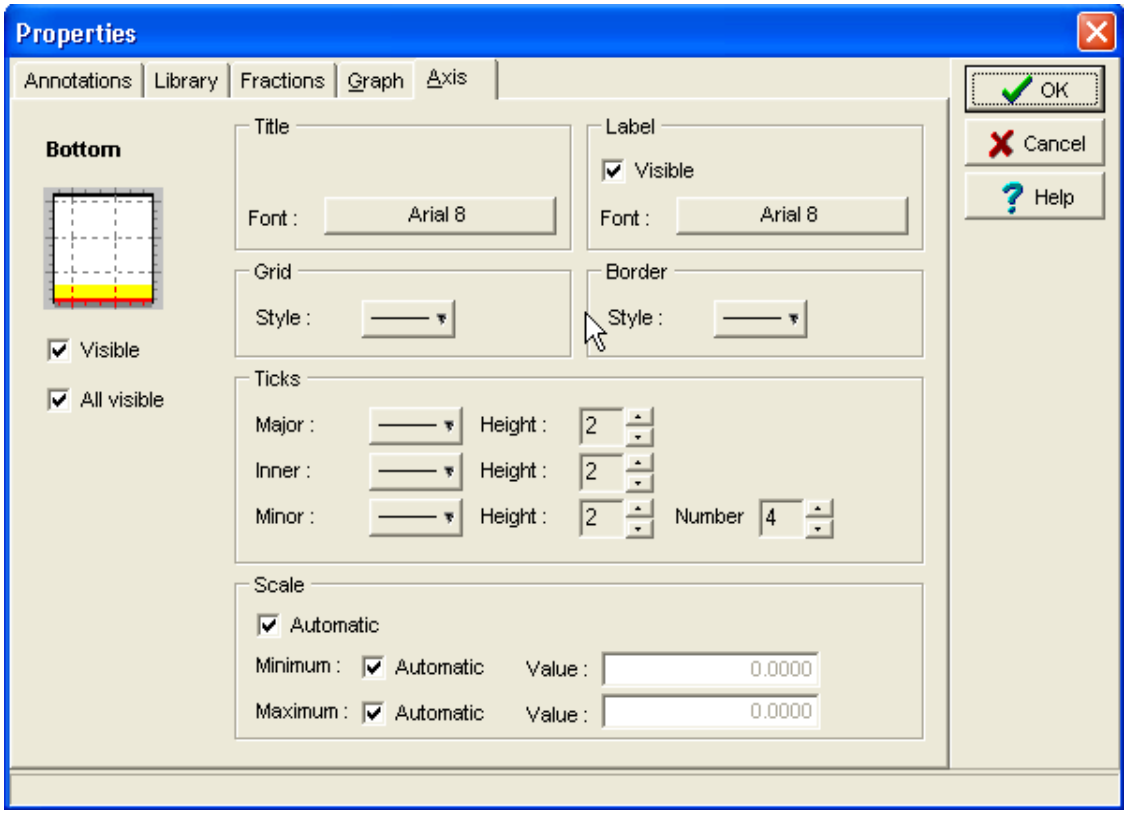
In the Curve properties, select the Graph tab.



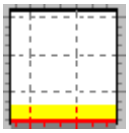
- In Margin Section, the interval between the curve and its border may be changed, as the percentages increase, the margin also increases.
- In Panning Section, check the box Right mouse button. Click and drag the right mouse button in the area of a graph, and the curve moves with the mouse (translation).
- Check the box Axis arrows. When the mouse is placed on an axis of the chromatogram, it takes the shape of an arrow. A left button click moves the curve in the arrow opposite direction. Change the % Scrolling value to choose the shifting length.
- Zoom Section: Check the box Animated to break down the zoom in as many steps as defined on the right of this check box.
- Check the box Zoom out with double-click, and the graph scale will be set as in the last zoom out action.
- The box Zoom in ratio is used to modify the speed of the zoom within the popup menu.
- Color Section: The background or frame colors can be changed by clicking on and then selecting the color of the background or the frame. Check graduation to obtain a graduated color effect for the graph frame.

Axis

In the Curve properties, select the Axis tab.



In the graph on the left, select (with a click) the axis to be configured:



The example above highlights the selected axis on the bottom (x-axis).

Now choose the parameters to configure the selected axis:

- Title:

Press the Font: Arial 8 button to select the font for the title of the curve.

- Label:

Press the Arial 8 button to select the axis font: the script, the height, the color, etc.

Uncheck the Visible box to hide the axis label.

Grid: Click on the arrow to modify the style of the graph grid and to show or hide it.

Border: Click on the arrow to modify the style of the graph border and to show or hide it.

Ticks: It is possible to modify the number of the ticks, their frequency, their length, etc.

The graphical properties are chosen only for the graph in which the right mouse button was pressed.

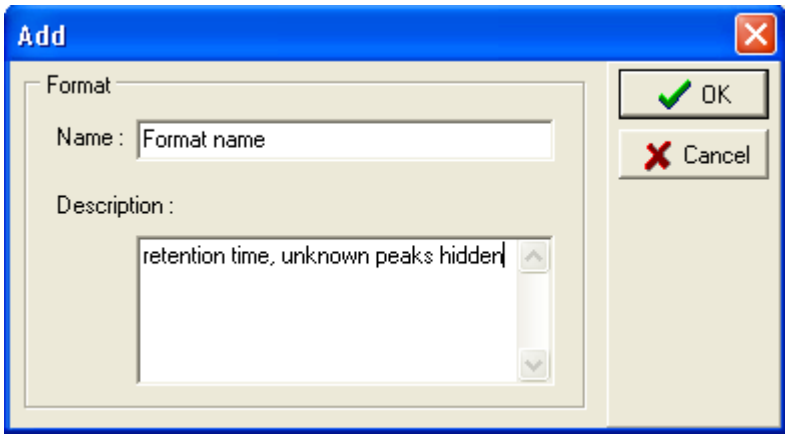
Library

Once chromatogram annotations and colors have been defined, it is possible to apply them for every new chromatogram. It is also possible to view the chromatogram with annotations, and then print it with a different set of annotations using the CompassCDS Report Editor. This is possible by using a saved chromatogram format.

The chromatogram annotations, graphic properties, and axis properties are saved in the chromatogram.

When all of these parameters are set correctly, the chromatogram format can be saved. In the chromatogram format, go to the ‘Library’ page and then press the ‘Save current format’ button.

Enter the name of the format in the window and a short description of the format in order to recognize it quickly:



Press OK and the format is added to all the other formats.

When a new method is defined, it is possible to apply an existing chromatogram format in the Format sub-method, press the ‘Edit’ button inside the chromatogram format, select ‘library’ tab in the corresponding format and apply it. To print the chromatograms with a special format, open the CompassCDS Report Editor, right click in the area of the chromatogram, select Properties, then select the name of the format in the top right hand corner of the window.

NOTE: The ‘Chromatogram name’ is always printed, whatever the corresponding option is checked or not in the library.

The Suitability Tests

The suitability tests allow the display of selected warnings if defined variables reach certain values. The tests can consider any variable available in the Variable editor (METHOD / VARIABLES).

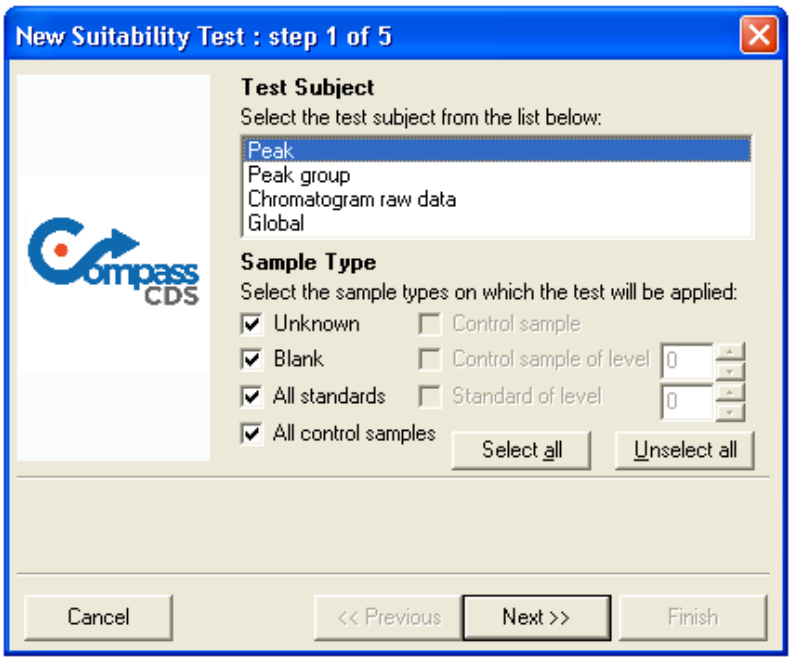
To display the suitability tests section of the method, select the menu METHOD / SUITABILITY TESTS or press the key combination Ctrl + T or select ‘Method’, then ‘Suitability’ in the browser.

Click on the Add button, then a 'Suitability test wizard' appears.

Suitability Test Wizard

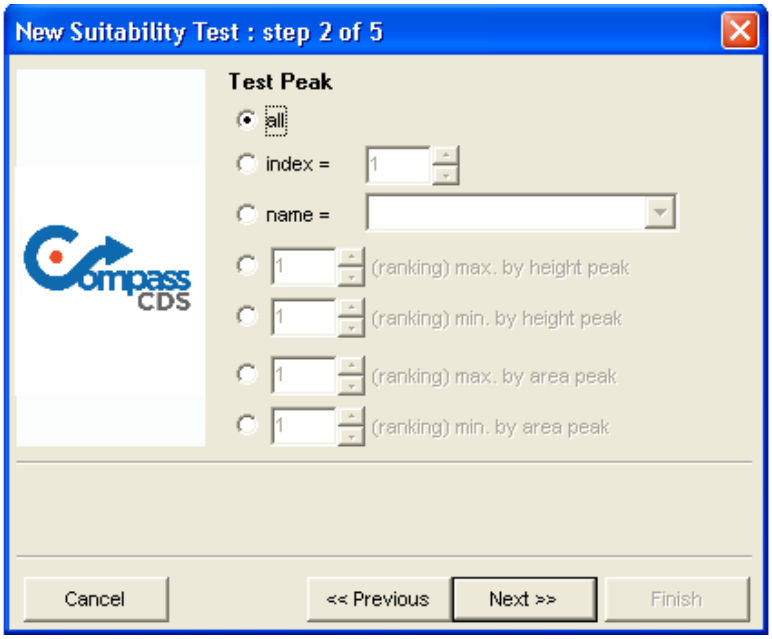
The wizard consists of several windows, which can be viewed using the NEXT and PREVIOUS buttons. When moving ahead within the wizard, text appears at the bottom of the screen, which lists what has been selected previously.

In the first window of the wizard, select the scope of the variable to be tested.



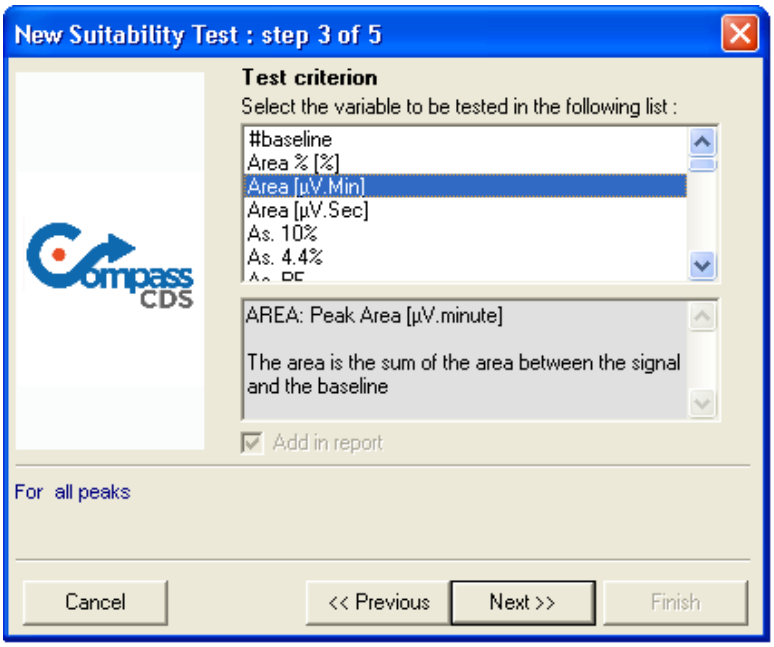
Choose to test either peak variables (quantity, area, asymmetry, etc.); or group variables (group quantity, group area, etc.); or chromatogram variables (sample mass, total area, etc., and all user input variables) or the chromatogram raw data (height of the signal). Precise the sample type concerned by the test: Unknown, blank, standard of a defined level or of all levels, control sample, control sample of a defined level or all control samples.

In the second window, choose the item to be tested.



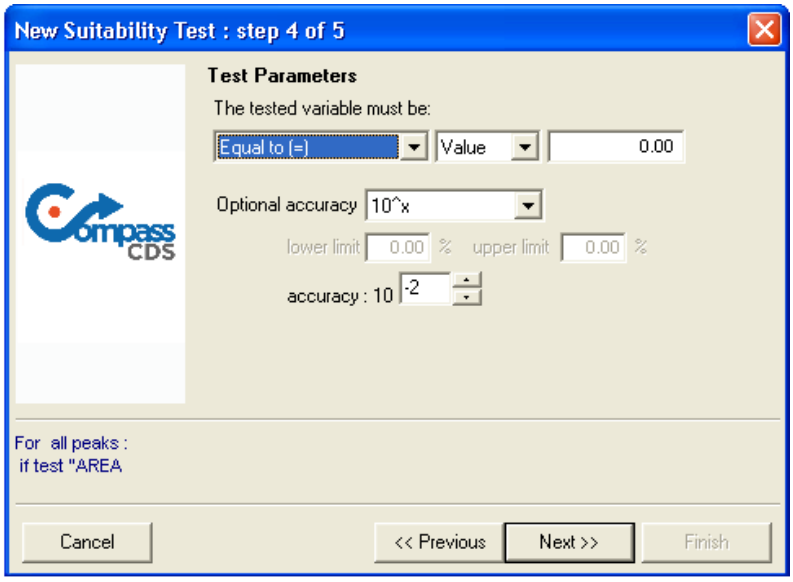
For example, if the tested variable is a peak or a group variable, choose if all the peaks or all the groups should be tested or choose the name, the index, etc., of the peak or group that should be tested. If the signal value is tested, choose which acquisition points (slice) must be tested: all the points (whole); the points between the x^{th} and the y^{th} acquisition points (Slices from x to y); or the points between x and y minutes (Time range from x to y min). If the variable is a global one (chromatogram variable) then this step is by-passed.

In the third window of the wizard, the tested variables are chosen:



The list of all the variables defined for the selected scope is displayed, including the user defined variable. Click on the variable to be tested and press the Next button. If the signal value is tested (raw data), choose to test either the minimum value of the signal between the two limits or the maximum value.

In the fourth step, choose the second part of the test.



The variable(s) can be defined as equal or different to a certain value or of another variable value, with a precision. The variable(s) can also be defined greater than or less than a certain value (strictly or not).

“Optional accuracy” settings:

Computers cannot handle precisely. Indeed there are some fractional values that cannot be represented at all, and if a calculation results in one of those numbers, then the result is the nearest Real number that it can provide. Which numbers those are depends on the precision of the number used.

CompassCDS uses Double precision but technically absolute accuracy is not possible. So, rather than an option of equality, one should really say “equal to or at least very near to” when dealing with Real numbers, which is exactly what “Accuracy” does, it give a small amount of lee-way in the equality check.

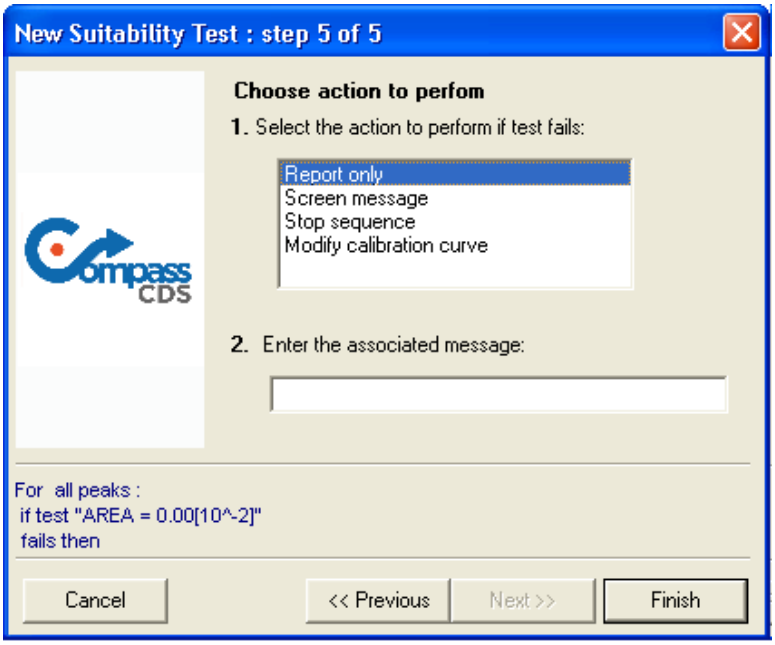
So, in the above setting the QTY of “Peak A” must be equal to 10.0, or at least within 10-2 of 10.0, i.e., 9.99 to 10.01. To increase the accuracy scroll the accuracy control to a more negative number.

This topic originally arose due to the desire to use a control sample to check the calibration. In this scenario one wouldn’t expect exactly the nominal value, but something close to it. Also, the above case presumes the desired value is in the middle of the allowed range, and this is not always the case. This is when the alternative setting of “Limits” can be used.

As can be seen, different lower and upper limits can now be set, as a percentage of the target value.

So in the above case, if the calculated concentration of any peak is within 99% to 102% of the defined level in the Control standard, the test will have deemed to have been passed, if the concentration is outside these limits, it will have failed.

In the last step, choose the action to perform if the test fails.



The user can define a message to display only in the printed report (Report only), or both in the printed report and on the screen (Screen message). The user can also decide to stop the sequence after the processing of the current chromatogram acquisition by choosing the 'Stop sequence' option. This option has a meaning only for suitability done during a sequence run. The Modify calibration curve action has to be used only if 'Control sample of level' is selected to realize the test. The action is that if the test failed all the calibration points of the same level than the one of the 'Control sample of level' that is tested are removed from the calibration curve and replaced by the unique point corresponding to the 'Control sample of level'.

By default, if a test is done on all the peaks, a new variable which result is either true or false is created. This variable can be displayed in the peak report. The name of this variable is SuitabilityX and it is possible to rename it in the variable editor. In the same way a group variable is created if a test is done on all the groups.

Press 'Finish' button in the last window to add the test. When the test is added, select it and press the button 'Edit test' or 'Edit action' to modify the test.

Suitability Test Examples

- **Peak asymmetry:** To test the peak asymmetry, add a suitability test. Choose Peak as the test subject, choose to test "All" peaks, choose As10% as the test criterion, choose between 0.9 and 1.1 as the test parameters. Then choose Report only as the result and press 'Finish'. In the peak report press the right-mouse button and choose Report properties and add a column for the suitability test.
- If you want to change the heading of the column, select the menu METHOD / VARIABLES. Search for the variable called 'Suitability 1' corresponding to the test and change the name to 'Asymmetry'.
- **Quantity of a component:** To test the quantity of a component (e.g. Benzene), add a suitability test. Choose Peak as the test subject, choose to test a peak selected with its name and select Benzene from the drop-down list, choose Qty as the test criterion, choose less than 15 as the test value. Then choose Report only as the result and enter a message saying 'Quantity of Benzene is superior to 15 ppm' for example and press OK. Now, in the

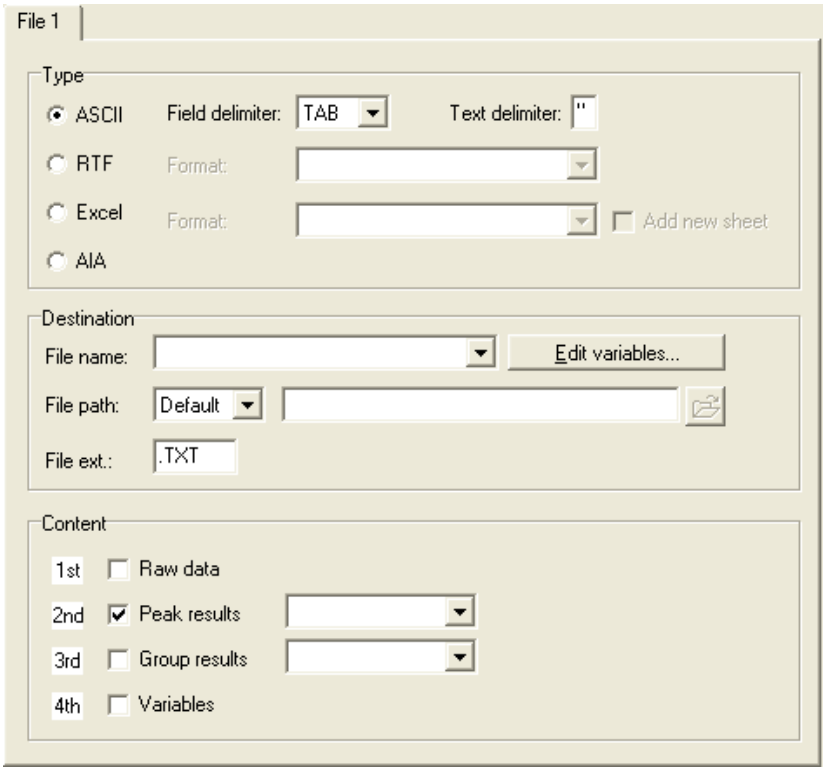
report style in the CompassCDS Report Editor, Add a Suitability result object to print the alarm if the test is negative.

To add a suitability test object in the CompassCDS Report Editor, press

Exporting the Results

It is possible to automatically export certain data (chromatogram, peak report or group report) in a defined format (Word, Excel, AIA, ASCII).

In the export section of the method, press the Add button and the following screen is displayed:



First choose the file type in which the results are to be exported: ASCII, Excel, AIA, or RTF

- **ASCII:** Choose the field delimiter that will separate the elements contained in a table. By default it is a tab, but choose “other” to delimit the text with any other character. Choose also the text delimiter that will enclose text fields.
- **Excel:** Select the version of the Excel program that will use the exported file.
- **AIA:** Export of level 3. This export contains raw data (point number, rate, etc.); peak data (result table, method name, peak variables, etc.); detection method parameters; sample description (mass, injection volume, information, etc.); administrative data (operator, data set origin, chromatogram title, etc.).
- **RTF:** Select the application in which the exported file will be read.

Then choose the file destination:

- **Name:** The name of the file can correspond to a variable. For example, choose Chromatoname from the list and the name of the exported file will have the name of the chromatogram with the chosen extension.

A special variable can be created to specify the file name. For example, click on ‘Edit variables’ and, within the Variable editor, create a new variable called ‘ExportName’. For example purposes, it will be a global variable, a string, defined with the following user formula: ‘Export_’+Chromatoname’. Now press the Apply button and select ExportName in the File name list box. In this case, if the chromatogram is called “chromato_1.data”, the name of the exported file will be “Export_ chromato_1.ext”.

To export a file for each channel when there are several channels in a method, define a variable whose formula will be ‘Chromatoname+Channelnumber’.

If variables have the same value in different chromatograms, the results can be exported to the same Excel file but in different worksheets. Check the box ‘Add new sheet’ in the export part of used method.

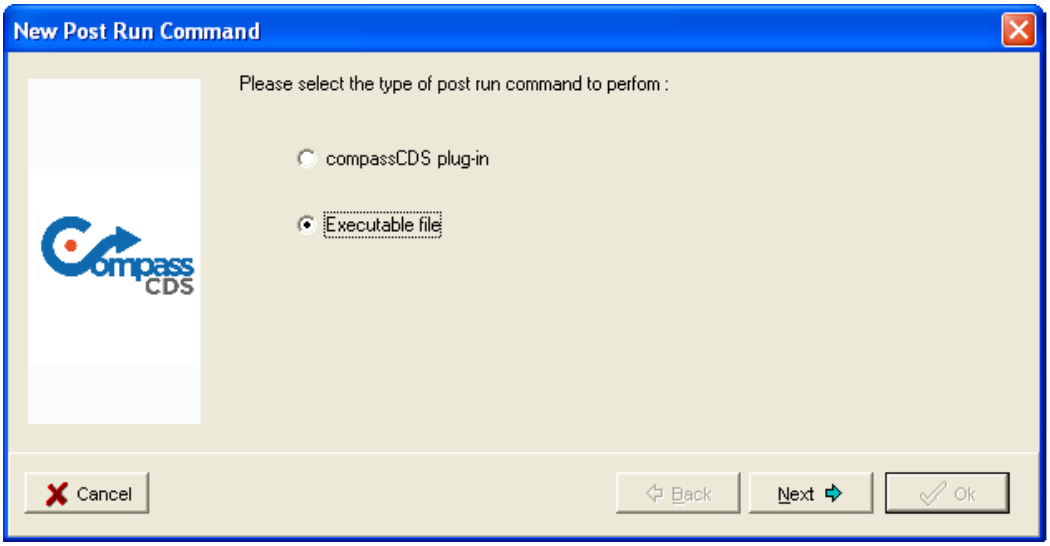
- **Path:** Choose the path of the directory in which the file will be exported. By default, the path will be the chromatogram path, but, if the Custom option is chosen from the drop list box, another path can be defined in next field.
- If the entered path does not exist, it is created during processing.
- **Extension:** By default, an extension corresponding to the file format will be defined, but it is possible to change it, e.g. defining a special format for a LIMS.
- Now choose the content of the exported file:
- **Raw data:** Check this box to export the raw data (the retention time and the absolute height of each point of the chromatogram). The raw data is always exported in the case of AIA export.
- **Peak results:** Check this box to export a peak table, which is the list of the chromatogram peaks. To define the format of this table, select the format of the peak table in the associated scrolling list (formats are created and detailed page 95). In case of AIA export, the format will be exported as it is defined in the current chromatogram results table
- **Group results:** Check this box to export a group table (the list of the groups). A format for this table may also be specified (as for peak results).
- **Variables:** Check this box to export all the global variables (the list of the global variables with their values).

Be careful to close the file before executing the processing. If the export file name is always the same and if you open it and start the processing, the export cannot be completed. In addition, if a file with the same name already exists, it will be overwritten without a warning message.

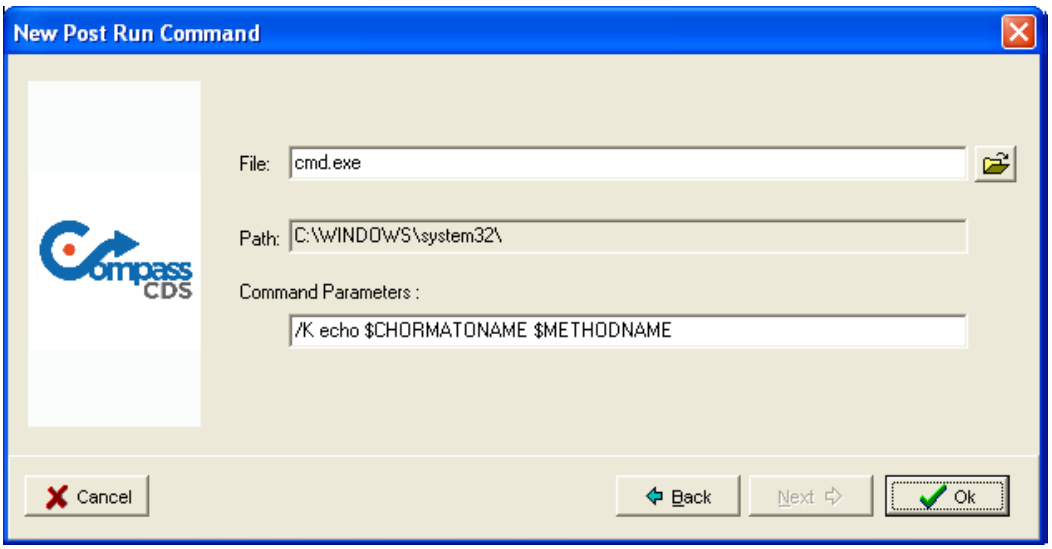
The Post Processing

This function allows the automatic execution of a program (Plug-In) using CompassCDS results.

Click on the add button, and then specify in the following screen whether the post processing is a plug in or an executable file.



If it is an executable file, the following screen is displayed:



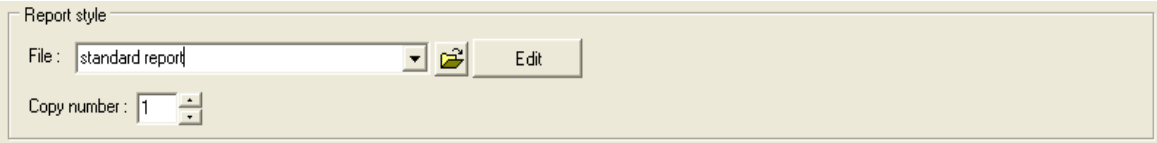
Select the executable file name in the ‘File’ field, the path is automatically displayed in the ‘Path’ field.

If the program to run needs some CompassCDS global variable(s) (system or user input variables) to be executed, the user has to define these variable names in the command parameters field. The syntax to use is ‘$’ and the ‘variable name’ (refer the variable chapter to know the name of the variables): $VARIABLEID1 $VARIABLEID2 etc.

According to the executable file chosen, a particular syntax can be used (see the example using the prompt command program where ‘/K echo’ is used to let the command prompt window open after the post processing has been executed.

Report Printing

The section ‘Report Style’ allows the user to define report printing. The following screen is displayed:



In the “File” box, select the name of the report template to print. Some templates must first be created in the CompassCDS Report Editor (see the corresponding user’s guide manual).

To view the selected report, press the Edit button: CompassCDS Report Editor is opened and displays the corresponding report template.

To print automatically a report after an acquisition, enter 1 in the “copy number” box. If 0 is selected, no printing will be done automatically.

The Summary Report

This function allows the user to generate a statistical report. All variables defined in CompassCDS can be statistically followed over time (retention time, RF, area, etc.). This is useful, e.g. for following column ageing by plotting the standard deviation of the retention time of a compound under specified analytical conditions.

This function is described in detail beginning on page 194.

Method Templates

Once a method has been built, it is possible to save it as a model in order to reuse it for the creation of new methods associated with other systems.

The methods created from a method template are the same as the original one except that the control section is not transferred.

Creating a Method Template

Once a method is created and saved, it is possible to save it as a template: Select this method and then the FILE / SAVE AS / SAVE METHOD AS TEMPLATE menu.

Now, you need to specify a name for the template method, be sure to enter a description of the template method in the corresponding field because this description will help you to identify it in the Open File window.

All the parameters of the mother method are saved in the template method, except the control parameters.

Creating a New Method using a method template

Select the menu FILE / NEW / NEW METHOD FROM TEMPLATE. Select the name of the template you would like to use and then select the system (chromatograph) the method should be applied to. A new method is created, using the model of the method template and with the default control parameters associated with the selected system.

This method can be manipulated as if it is a newly created one.

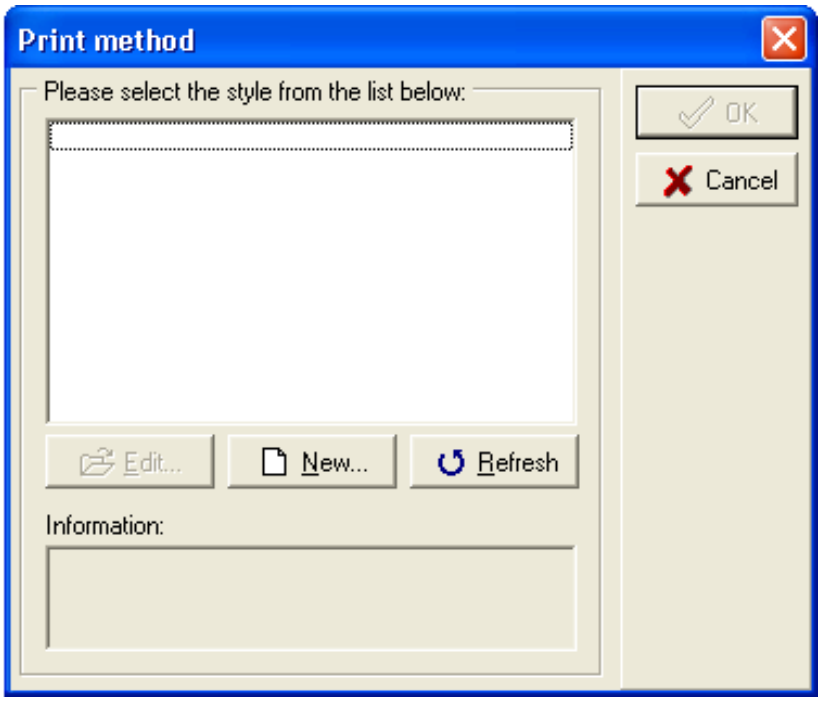
Do not forget to enter the parameter values in the control section.

Template Method Path

The templates methods are saved in a specific path, common to a group. This path is specified in the CompassCDS Configuration Manager and can be different from the data path.

Printing Method Parameters

To print method parameters, open it, and then click on the icon. The following screen is displayed:



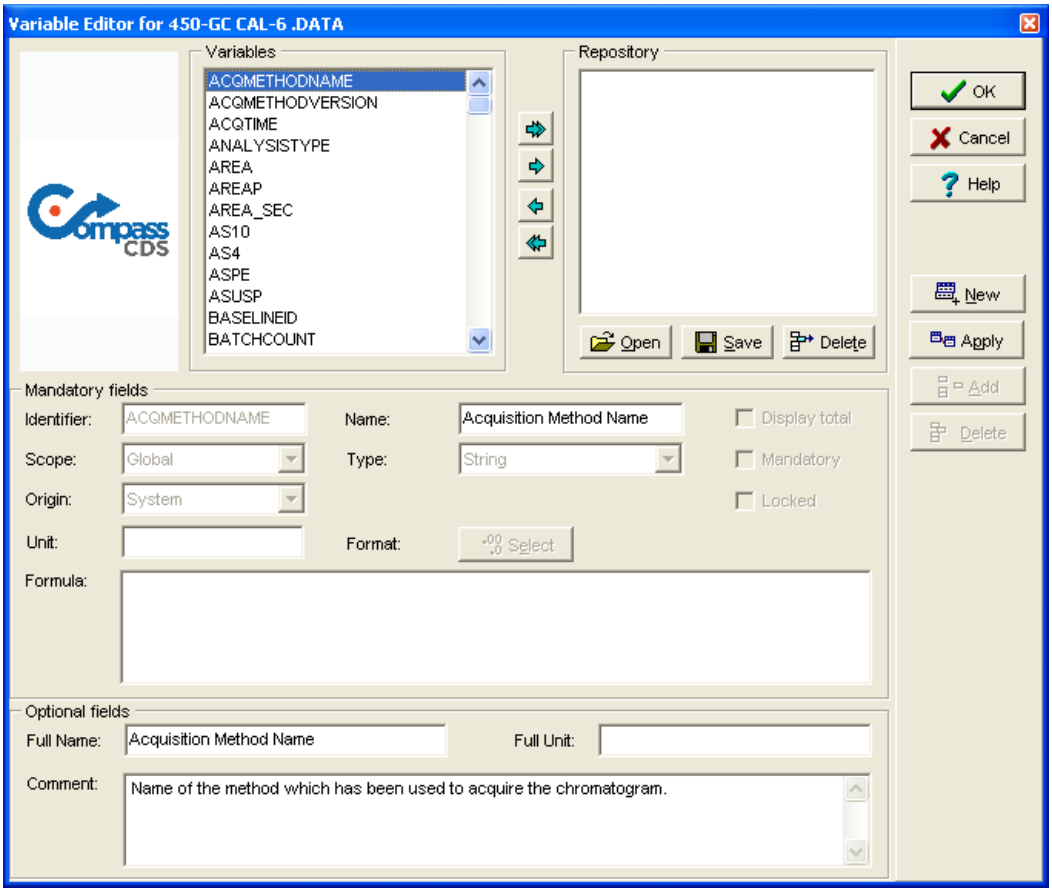
When the user selects a defined report in the list, he can edit it by pressing the Edit button; create a new one by pressing the ‘New’ button to customize the report, or refresh the list by pressing the ‘Refresh’ button.

CompassCDS Variables

CompassCDS incorporates many system variables that can perform calculations on individual peaks, peak groups, or the entire sample. It can also offer the possibility to define custom variables for calculations, which are not present by default in the existing CompassCDS variables. These can be either ‘user input’ variables for which the user must enter a value or text, or ‘user formula’ variables which allow specific calculations.

The variables are saved as part of the current method.

The management of the variables is done in the CompassCDS Variable Editor, available from the METHOD / VARIABLES menu:



The Variable Editor is composed of several parts, detailed in this manual:

- Variable list
- Repository
- Variable definition parameters

And specific buttons:

New: Creation of a new variable

Apply: Apply the changes made for the selected variables

Add: Save a variable with another name (remind to change the identifier)

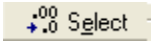
Delete: Delete the selected non-system variable

How a Variable is Defined

A variable is defined by the following elements:

- **Identifier:** The identifier is a short name to identify the variable. It can be used to print the variable in the CompassCDS Report Editor or be used to insert the variable into the formula of another variable. An identifier must be composed of letters, numbers or underscores. The first character of an identifier should be a letter.
- **Name:** The name of the variable is used to identify the variable into the software. For peak variables, the name is used in the peak result table (column heading), and also in the peak

results object in the CompassCDS Report Editor reports. For group variables, the name is used in the group report. For global variables, the name is used in the CHROMATOGRAM PROPERTIES. The name of the standard variables can be modified.

- **Unit:** The abbreviation of the unit of the variable. It is indicated in the heading of the peak or group report, or in the CHROMATOGRAM PROPERTIES after the name of the variable. The unit of standard variables can be modified.
- **Scope:** The scope is used to define if the variable applies to a peak, peak group, or the entire sample. For example, Area and Quantity can apply to peaks or groups, and sample weight is global. Peak variables can be displayed in the peak report; group variables can be displayed in the group report, while global variables are displayed in chromatogram properties (menu options DATA / CHROMATOGRAM PROPERTIES).
- **Type:** The type of a variable can be a real number, an integer, a string of characters or Boolean. A Boolean is defined by a condition in a formula (see below). If the condition is satisfied, the value of the Boolean is TRUE, otherwise, it is FALSE. It is possible to modify the type of a variable. To transform a real into an integer, use 'Trunc' or 'Round'. To transform a string into a real, use 'Float'. To transform a real into a string, use 'String' (see the 'Usual Functions' chapter, page 134).
- **Default value:** This field is accessible only for non-mandatory user input variables ('global' and 'by peak'). It allows entry of a default value.
- **Origin:** The origin of a variable depends on the way in which the value of the variable is obtained. For a standard variable, the origin of the variable will be 'System'. User- defined variables can be calculated with a formula ('User formula'). The user can also edit them in the acquisition windows (Quick Start or sequences) or in the CHROMATOGRAM PROPERTIES if the origin is 'User input'.
- **Display total:** This box is active only for group and peak variables. Check this box if the variable is to be summed for all the peaks or groups. The total will appear at the bottom of the peak or group report.
- **Mandatory variables:** This box is active only for 'User input' variables. By checking this box, CompassCDS will refuse to launch an acquisition if the variable has not been entered (in Quick Start window or the sequence).
- **Locked:** This option is available only if the user owns the corresponding profile. The user input variable may be locked so other users may not change it.
- **Format:** Press the Format button 

to define the display format of the real numbers. Three types of formats exist: automatic, scientific, and fixed. Choose the number of decimals to be displayed. For example, for the area variable, select scientific with a precision of 5, and the area of a peak displayed will be '4.18345e4'. If fixed is selected with a precision of 3, the same area will be displayed as '4183.452'. Automatic mode is the same as fixed mode, but with comma separation at each thousand. The format may be modified for standard variables.
- **Formula:** This field is accessible only for User formula variables. It allows the definition of the calculation formula of the variable (see the' How to Express the Formula' chapter, page 131).
- **Full name:** The full name of the variable is given in this area. This full name appears only in this window. It provides information related to the content of the variable.
- **Full unit:** The full name of the unit is given in this area. This full unit appears only in this window. It provides information related to the unit of the variable.
- **Comment:** A comment that explains the calculations of the variable, its origin, or any other useful information. This information cannot be modified for system variables.

For the system variables, it is only possible to modify the full name and the format.

System Variables

The system variables are defined by default in CompassCDS. As mentioned in the previous paragraph, a variable is defined by an Identifier and a Name. In this section, all the system variables are described and listed by their Name and Identifier under the following syntax: Name [IDENTIFIER].

Peak System Variables

The peak system variables can be displayed in the peak report. (Choose REPORT FORMAT in the popup menu and select the variables for report display).

CompassCDS calculates the following variables automatically for each peak:

Retention Time

- **Corrected time** [min**] [RTCORRECT]:** Theoretical retention time (from the identification table) corrected according to the retention times of reference peaks. For example, if a peak was expected at 9 minutes between two reference peaks expected at 8 and 10 minutes, and the reference peaks occur at 8.5 and 10.5 minutes, the corrected retention time of the peak will be 9.5 minutes (See “Identification” section).
- **RT. Index [RTINDEX]:** This is an index giving the position of the peak between the two adjacent reference peaks: If the two adjacent reference peaks are the nth and the n+1th reference peaks, the RT index of the peak equals:

$$\text{index} = \frac{\text{Rt} - \text{Rt}_n}{\text{Rt}_{n+1} - \text{Rt}_n} + n$$

Where

Rt is the peak retention time.

Rtn is the retention time of the previous reference peak.

Rt_{n+1} is the retention time of the next reference peak.

- **RT Offset** [min] **[OFFSET]:** This parameter is calculated for identified peaks and is the difference (in minutes) between the theoretical retention time of the peak and its actual retention time. The theoretical retention time is the time set in the identification table.
- **Start** [min] **[RTSTART]:** Time at the beginning of the peak (in minutes). It corresponds to the time of the peak start marker (or if the marker is a valley).
- **Stop** [min] **[RTSTOP]:** Time at the end of the peak (in minutes). It corresponds to the time of the peak stop marker (or if the marker is a valley).
- **Time** [min] **[RT]:** Retention time at the peak apex (in minutes).

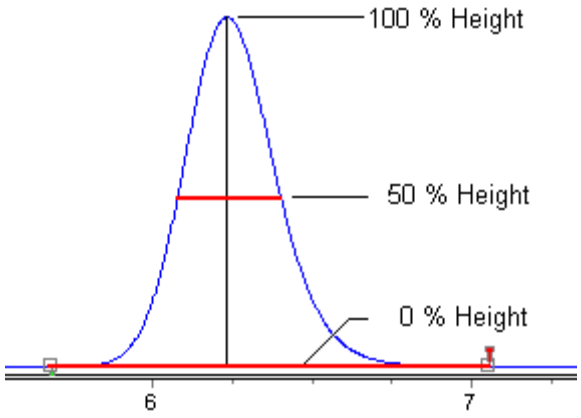
Response

- **Area** [µV.min] **[AREA]:** The area is the sum of the area between the signal and the baseline between the two peak edges (peak start and end markers).
- **Area** [µV.sec] **[AREA]:** The area is the sum of the area between the signal and the baseline between the two peak edges (peak start and end markers).
- **Area** [%] **[AREAP]:** The area percentage is the area of the peak divided by the sum of the areas of all the peaks, multiplied by 100.

- **Height** [µV] **[HEIGHT]:** The height is the difference between the value of the signal at the apex of the peak and the value of the baseline at the same time.
- **Height** [%] **[HEIGHTP]:** The height percentage is the height of the peak divided by the sum of the heights of all the peaks, multiplied by 100.
- **Recomputed RF [RF_Rec]**: This is the recomputed response factor. It is equal to the ratio between the quantity calculated by CompassCDS and the response.
- **Recomputed RRF [RRF_Rec]:** This is the recomputed inverse response factor. It is equal to the inverse of the Recomputed Response Factor.
- **Response [RESP]:** The response is either the area, the height, the area% or the height%, the area$^{1/2}$ and the height$^{1/2}$ according to the choice made in the calibration method (response section).
- **RF [RF]:** This is the response factor entered in the calibration table (in the case of a calibration with manual response factors) or the ratio of the quantity (read from the calibration curve) of the peak by its response (in the case of calibration with a calibration curve).
- **RRF [RRF]:** This is the inverse response factor. RRF = 1/RF= Response / Quantity.

Width

- **Width X%** [min] **[WX]:** The width of the peak measured at the specified height (X). The height is expressed as a percentage of the total height of the peak. 0% of the height is on the baseline, 100% of the height is on the top of the peak:



A height of 4.4% corresponds to the 5-sigma method

A height of 13.4% corresponds to the 4-sigma method

A height of 32.4% corresponds to the 3-sigma method

A height of 60.7% corresponds to the 2-sigma method

Seven heights are proposed:

X= 4 means 4.4 %

X= 5 means 5 %

X= 10 means 10 %

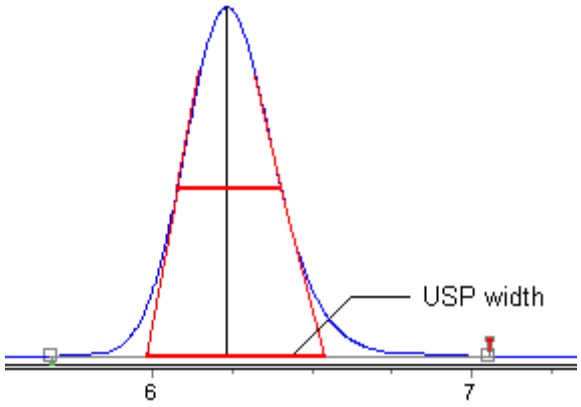
X= 13 means 13.4 %

X= 32 means 32.4 %

X= 50 means 50 %

X= 60 means 60.7 %

- **Width USP** [min] **[W_USP]:** Peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.



- **Left Half Width X%** [min] **[WLX]:** Left half peak width measured at the specified height (X).The height is expressed as a percentage of the total height of the peak. 0% of the height is on the baseline, 100% of the height is on the top of the peak:

Seven heights are proposed:

X= 4 means 4.4 %

X= 5 means 5 %

X= 10 means 10 %

X= 13 means 13.4 %

X= 32 means 32.4 %

X= 50 means 50 %

X= 60 means 60.7 %

- **Left Half Width USP** [min] **[WL_USP]:** Left half peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.

Asymmetry

- **As.PE. [ASPE]:** Asymmetry calculated with the European Pharmacopoeia method:

$$A_s = \frac{W_{5\%}}{2 * W_{1/2}}$$

Where

W5% is the peak width at 5% of peak height.

W1/2 is the first half-width at 5% of peak height.

- **As.USP. [ASUSP]:** Asymmetry calculated with the United States Pharmacopoeia method:

$$A_s = \frac{W_{5\%}}{2 * f}$$

Where

W5% is the peak width at 5% of peak height.

f is the first half-width at 5% of peak height.

- **As.EMG/ASTM [ASUSP]:** EMG and ASTM methods for Asymmetry calculation are the same as the United States Pharmacopoeia method.
- **As. 4.4% [AS4]:** It is a half-width method:

$$A_s = \frac{W_{2/2}}{W_{1/2}}$$

Where

W1/2 is the first half-width at 4.4 % of peak height.

W2/2 is the second half-width at 4.4 % of peak height.

- **As. 10% [AS10]:** It is a half-width method:

$$A_s = \frac{W_{2/2}}{W_{1/2}}$$

Where

W1/2 is the first half-width at 10 % of peak height.

W2/2 is the second half-width at 10 % of peak height.

Number of Theoretical Plates

- **NTP Sx [NTP_SX]:** This is the number of theoretical plates calculated with the x-sigma method:

$$NTP = R_{sigma}\left(\frac{R_t}{w}\right)^2$$

Where

Rt is the peak retention time.

w is the peak width at the height corresponding to the calculation method:

R_{sigma} is a factor which depends on the calculation method:

5 sigma method: R_{sigma} = 25, width measured at 4.4 % of peak height

4 sigma method: R_{sigma} = 16, width measured at 13.4 %

3 sigma method: Rsigma = 9, width measured at 32.4 %

2 sigma method: Rsigma = 4, width measured at 60.7 %

- **NTP USP [NTP_USP]:** This is the number of theoretical plates calculated with the United States Pharmacopoeia method:

$$NTP = 16 \times \left(\frac{R_t}{w} \right)^2$$

Where

Rt is the peak retention time

w is the USP Width (peak width measured at peak base, by extrapolating the tangents of the peak sides. The tangents are taken at the inflection points of the sides.)

- **NTP EP [NTP_EP]:** This is the number of theoretical plates calculated with the European Pharmacopoeia method:

$$NTP = 8\mathrm{Ln}(2)\left(\frac{R_t}{w} \right)^2$$

Where

Rt is the peak retention time.

w is the peak width measured at the half peak height.

- **NTP JP/ASTM [NTP_EP]:** JP and ASTM methods for theoretical plate's number calculation are the same as European Pharmacopoeia method.
- **NTP EMG [NTP_EMG]:** This is the number of theoretical plates calculated with the EMG method:

$$NTP = 41.7 \times \frac{\left(\frac{R_t}{W_{10\%}} \right)^2}{\frac{W_{1/2-10\%}}{W_{2/2-10\%}} + 1.25}$$

Where

Rt is the peak retention time

W10% is the peak width measured at 10% of peak height.

W1/2-10% is the first half peak width measured at 10% of peak height.

W2/2-10% is the second half peak width measured at 10% of peak height.

- NTP AH [NTP_AH]: This is the number of theoretical plates calculated with the Area/Height method:

$$NTP = 16 \times \left(\frac{R_t}{4 \times 0.399 \times \left(\frac{A}{h} \right)} \right)^2$$

Where

Rt is the peak retention time

A is the area of the peak in µV.min.

h is the height of the peak in µV.

Selectivity, Capacity

- **α[SEL]:** This is the selectivity factor, which is the ratio of the peak capacity factor (k') to the capacity factor of the previous peak:

$$\alpha = \frac{k_2}{k_1} \quad \text{or} \quad \alpha = \frac{Rt_2 - T_0}{Rt_1 - T_0}$$

Where

T_0, Rt_1 and Rt_2 represent respectively the dead time, the peak retention time of the previous peak and the retention time of the current peak.

The dead time, T_0, set in the acquisition window (Quick Start or sequence), can be modified in the chromatogram properties (Menu DATA / CHROMATOGRAM PROPERTIES).

- **k' [KP]:** the capacity factor (k') of a compound is the ratio of the quantities of the compound in the stationary phase and in the mobile phase.

$$k' = \frac{Rt - T_0}{T_0} = \frac{qstat}{qmob}$$

Where

T_0 and Rt represent respectively the dead time and the peak retention time, qstat the quantity of the compound in the stationary phase and qmob the quantity of the compound in the mobile phase.

Resolution

The resolution quantifies the integrity of the separation between two successive peaks.

- **Res. HW [RES_HW]:** This is the resolution calculated with the half width method:

$$R_s = 1.18 \times \frac{Rt_2 - Rt_1}{W_1 + W_2}$$

Where

Rt_2 and Rt_1 represent respectively the peak retention time and the retention time of the previous peak.

W_1 is the half height width of the first peak.

W_2 is the half height width of the second peak.

- **Res. EMG/EP/ASTM [RES_HW]:** EMG, European Pharmacopoeia, and ASTM resolutions are calculated as half width Resolution.

- **Res. USP [RES_USP]:** This is the resolution calculated with the United States Pharmacopoeia method:

$$R_s = 2 \times \frac{Rt_2 - Rt_1}{w_1 + w_2}$$

Where

Rt_1 and Rt_2 represent respectively the peak retention time of the previous peak and the retention time of the current peak.

W_1 is the USP width of the previous peak.

W_2 is the USP width of the current peak.

See the section on Peak width for how USP width is calculated.

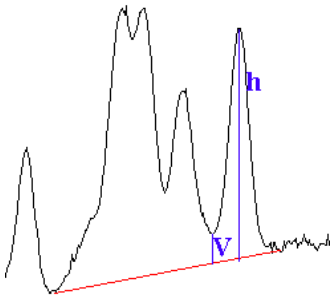
- **Res. Val. [RES_VAL]:** This is the resolution calculated with the valley method:

$$R = \frac{V}{h}$$

Where

V is the height of the valley preceding the peak.

h is the height of the peak.



Name, Quantities

- **Control sample [CTRLSAMPLE]:** It is the quantity entered in the calibration table for the control sample. This value is used for the control sample computation.
- **Name [NAME]:** The name assigned to the peak after the identification (See “Identification” section). The name is used to quantify the peak if the calibration mode is different from response percentages.
- **Qtable [QTABLE]:** Quantity entered in the calibration table for the peak and the corresponding chromatogram level, if the chromatogram is a standard or a control sample with level.
- **Quantity [unit] [QTY]:** The quantity of the peak (See Quantification section).

Integration Code [CODE]

The integration code describes the way in which the baseline is drawn. The first letter describes the baseline position at the peak start and the second letter the baseline position at the peak end.

Possible cases:

S The baseline is on the signal.

H The baseline is horizontal.

V The end or the start of the peak is a valley.

T The peak is a shoulder, the baseline is tangential.

E The peak is a shoulder, the baseline is exponential.

M The peak has been integrated manually.

F The end or the start of the peak has been forced.

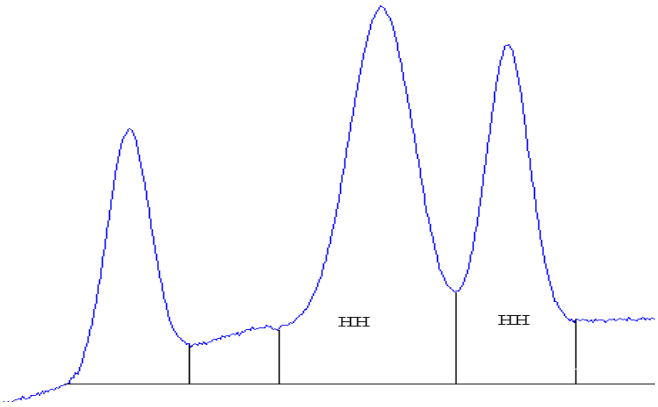
OR When the peak is saturated (Out of Range).

Priority rules:

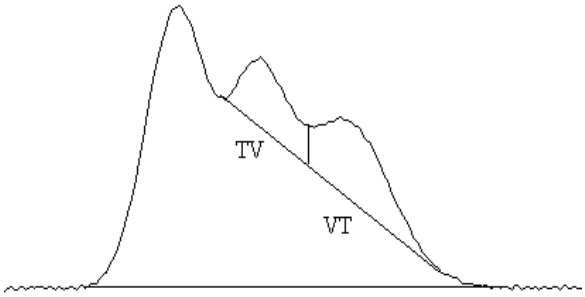
1. H has priority over S and V.
2. E and T can be replaced by V.
3. F has priority over H, S, V.
4. M has priority over F, H, S, V, E and T.
5. E and T have priority over S.
6. OR has priority over F, H, S, V, E and T.

Integration examples:

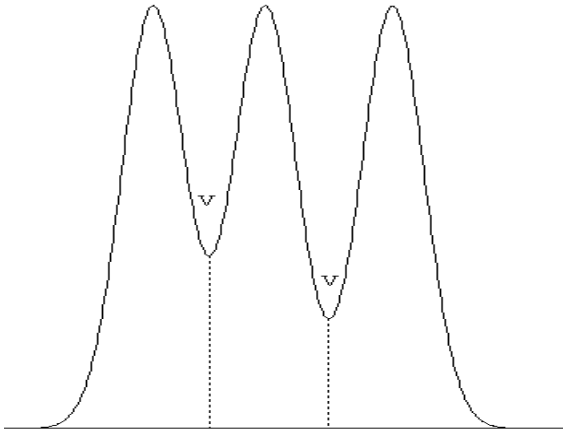
1. The baseline has been forced (rule 1).



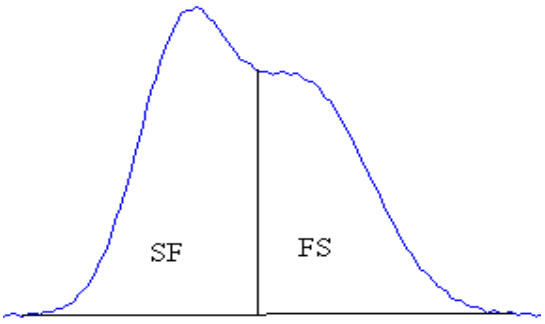
2. Two peaks integrated as tangential shoulders of a main peak (rule 2).



3. Integration ‘Valley to Valley’.



4. Forced integration: split peak.



It is also possible to indicate the saturation of a peak thanks to this variable. The associated code is OR (out of range). User has to enter the minimum and maximum value of the output signal (of the chromatograph) in the METHOD / INTEGRATION / PARAMETERS menu.

Saturation

Saturated [ISSAT]: This variable displays TRUE if the corresponding peak is saturated, FALSE in the other case according to the minimum and maximum values of the output signal (chromatographic signal) defined in the METHOD / INTEGRATION / PARAMETERS menu.

Moments, Excess (or Kurtosis), Skew

- **Moment1 [MOMENT1]:** The first moment of a peak is the mean retention time, which is the retention time of the peak at the center of gravity. It is referenced to the peak retention time (m1 is the time between the top and the center of gravity of the peak).

$$m_1 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)h_t dt$$

Where

m0 is the zero moment, or the peak area.

Rt the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

In the case of a Gaussian peak, m1 is equal to zero.

- **Moment2 [MOMENT2]:** The second moment of a peak is the variance 2σ (σ is the peak standard deviation). The second moment is a measure of the lateral spread.

$$m_2 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^2.h_t dt$$

Where

m_0 is the zero moment or the peak area.

R_t is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

- **Moment3 [MOMENT3]:** The third moment of a peak describes vertical asymmetry, or skew. It is a measure of the departure of the peak shape from the Gaussian standard.

$$m_3 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^3.h_t dt$$

Where

m_0 is the zero moment or the peak area.

Rt is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

In the case of a Gaussian peak, m_3 is equal to zero.

- **Moment4 [MOMENT4]:** The fourth moment (or excess) of a peak is a measure of the compression or stretching of the peak along a vertical axis, and how this compares with a Gaussian standard.

$$m_4 = \frac{1}{m_0}\int_{-\infty}^{+\infty}(t - R_t)^4.h_t dt$$

Where

m_0 is the zero moment, or the peak area.

Rt is the retention time of the peak.

t is the retention time of a slice.

h_t is the height of a slice.

dt is the acquisition period (the inverse of the number of acquisition points per minute).

- **Excess or Kurtosis [KURTOSIS]:** Excess is equal to zero for Gaussian peaks. E is negative for overloaded peaks.

$$E = \frac{m_4}{m_2^2} - 3$$

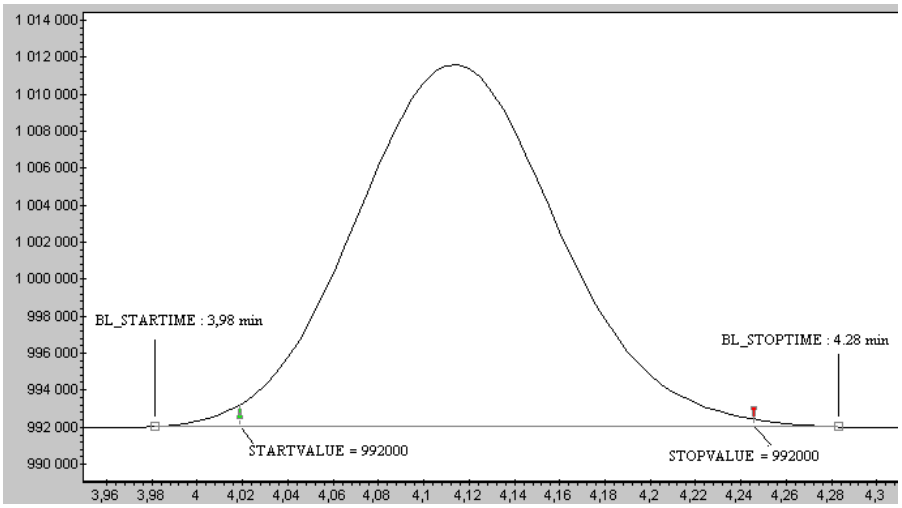
- **Skew [GAMMA]:** γ quantifies the symmetry of a peak.

$$\gamma = \frac{m_3}{m_2^{3/2}}$$

A symmetrical peak has a skew of zero, whereas a peak that tails has a positive skew and a peak that fronts has a negative skew.

Others

- **# Baseline [BASELINEID]:** Peak Baseline Identifier: Index of the peak baseline
- **Baseline Start Time [BL_STARTIME]:** Time of the start marker of the baseline.
- **Baseline Stop Time [BL_STOPTIME]:** Time of the stop marker of the baseline.
- **Baseline Start Value [BL_STARTVALVUE]:** Value of the signal of the baseline at the start peak time.
- **Baseline Stop Value [BL_STOPVALUE]:** Value of the signal of the baseline at the stop peak time.



- **Group(s) [PEAK_GROUP]:** Peak Group(s): The name(s) of the group(s) this peak belongs to.
- **Is Unknown [ISUNKNOWN]:** This variable equals TRUE if the peak is unknown (namely has not been identified) or FALSE if not.
- **Manual RF [ISRFMANUAL]:** This variable is TRUE if the peak has been calibrated in manual mode. Otherwise, it is FALSE.
- **Positive [ISPOS]:** This variable equals TRUE if the peak is a positive peak or FALSE if not.
- **Regression model [REGRMODEL]:** The regression model of the calibration curve used for peak quantification.
- **Response factor_relative standard deviation [RF-RSD]:** Expressed in percent. Obtained by multiplying the RF-SD by 100 and dividing the product by the RF of the associated calibration curve.
- **Response factor_standard deviation [RF-SD]:** Measures the dispersion of the response factors of the different points in the associated calibration curves.
- **Weighting factor [WEIGHTFACTOR]:** The weighting factor applied to the calibration curve used for peak quantification.

Group System Variables

The group variables can be displayed in the group result table. Select ‘report Properties’ in the popup menu of the group result table and select the variables to display. It is possible to save the group report formats as the peak report formats in a library, see page 101).

CompassCDS calculates the following variables for each peak group:

- **Area [µV.min] [G_AREA]** The area is the sum of the areas of all peaks in the group.
- **Area [%] [G_AREAP]:** The area percentage is the area of the group divided by the sum of the areas of all the groups, multiplied by 100.
- **Control sample [G_CTRLSAMPLE]:** Quantity entered in the calibration table for the control sample. This value is used for the control sample computations.
- **Height [µV] [G_HEIGHT]:** The height is the sum of the heights of all peaks in the group.
- **Height [%] [G_HEIGHTP]:** The height percentage is the height of the group divided by the sum of the heights of all the groups, multiplied by 100.
- **Manual RF [G_ISRFMANUAL]:** This variable is TRUE if the group has been calibrated in manual mode. Otherwise, it is FALSE.

- **Name [G_NAME]:** Group Name: Name of the group after identification
- **Number of peaks [G_NBPEAKS]:** The number of peaks included in a group.
- **Quantity** [unit] **[G_QTY]:** The quantity of the group. It equals the sum of the quantity of the group peaks.
- **Qtable** [unit] **[G_QTABLE]:** The Quantity entered in the calibration table for the group and for the corresponding chromatogram level if the chromatogram is a standard or a control sample with level.
- **Recomputed RF [G_RF_Rec]:** It is the recomputed response factor of the group.

For calibration group, if 'curve' factor is used: the response factor is the ratio of the quantity (read in the calibration curve) of the group by its response. If 'manual' factor is used: it is the ratio of the quantity calculated without M, D, mass or Normalization factor, by its response.

For result group, it is the ratio of the quantity calculated without M, D, mass or Normalization factor, by its response.

- **Recomputed RRF [G_RRF_Rec]:** It is the recomputed reverse response factor of the group. It is the reverse of the Recomputed Response Factor of the group.
- **Regression model [G_REGRMODEL]:** The regression model of the calibration curve used for group quantification.
- **Response [G_RESP]:** The response is either the total area, the height, the area% or the height%, the area$^{1/2}$ and the height $^{1/2}$ of the group, according to the choice made in the calibration method.
- **Response factor relative standard deviation [G_RFRSD]:** The response factor relative standard deviation is expressed in percent. It is obtained by multiplying the RF-SD by 100 and dividing the product by the RF of the associated calibration curve.
- **Response factor standard deviation [G_RFSD]:** The response factor standard deviation Measures the dispersion of the response factors of the different points in the associated calibration curve.
- **RF [G_RF]:** This is the response factor of the group. The response factor can be entered in the calibration table if the group is a calibration group, or it is the ratio of the quantity of the group to its response.
- **RRF [G_RRF]:** It is the inverse response factor of a group: RRF = 1/RF= Group response / Group quantity.
- **Weighting factor [G_WEIGHTFACTOR]:** The weighting factor applied to the calibration curve used for group quantification.

Global System Variables

The global variables belong to the whole chromatogram. They can be displayed in the chromatogram properties. Select the menu options DATA / CHROMATOGRAM PROPERTIES in the main menu.

Output Variables

CompassCDS Chromatography Data System automatically computes the following variables for each chromatogram:

- **# id. Peaks [NBIDPEAKS]:** Number of peaks defined in the peak identification tale.
- **Acquisition Method Name [ACQMETHODNAME]:** Name of the method used to acquire the chromatogram.

- **Acquisition Method Version [ACQMETHODVERSION]:** Version of the method used to acquire the chromatogram.
- Acquisition Date & Time [ACQTIME]: Acquisition date and time.
- **Calibration curve [CALNAME]:** The name of the calibration file associated to the chromatogram. If no curve, the value is an empty string.
- **Calibration type [CALTYPE]:** The type of calibration. The variable equals 0 if working in 'Response %', 1 in 'Normalization', 2 in 'External Standard', 3 in 'Internal Standard'.
- **Channel number [CHANNELNUMBER]:** A sample can be acquired on several channels, and a chromatogram is drawn for each channel. This variable gives the channel number of the chromatogram that is selected.
- Chromatogram Name [CHROMATONAME]: The name of the chromatogram.
- **Data path [DATAPATH]:** The data path of the currently connected user. This is the path of the directory containing the files, which is accessible by the current user.
- **Data saved [DATASAVED]:** This variable equals "True" if the chromatogram has been saved or "False if there were changes since the last time the chromatogram was saved. This variable can be used for mapping purposes: if the value of this variable is printed and should equal 'Yes', this will ensure that all the results that are printed are saved, and thus that there is a record of them and the way in which they were obtained.
- **Detector name [DETNAME]:** The name of the detector of the current channel.
- **Drift [DRIFT]:** This variable is the slope (a) of the regression straight line y=ax+b calculated with the "Compute noise On" and Off events (see noise variable).
- **Fraction collection log name [FRACLOGNAME]:** The name of the Log file associated to the chromatogram.
- **Fraction collection unit [FRACUNIT]:** The unit defined for the fraction collection (time, slope, level, etc.).
- **Group Name [GROUPNAME]:** The name of the connection group (defined in the CompassCDS Configuration Manager) on which the user has performed the last chromatogram processing.
- **# Groups [NGROUPS]:** The number of groups defined in the chromatogram.
- **#Int.Std.Peaks [ISTDNB]:** The number of internal standards defined in the method.
- **Injector name [INJECTORNAME]:** The name of the injector used for the acquisition.
- **Last calibration date [CALDATE]:** The last modification date of the calibration curve used to process the chromatogram.
- **Level [LEVEL]:** The calibration level if the chromatogram is a standard or 0 if it is an unknown.
- **Method channel [METHODCHANNEL]:** The name of the channel of the method file used to process the chromatogram.
- **Method name [METHODNAME]:** The name of the last method used to process the chromatogram.
- **Noise [NOISE]:** This variable is calculated between limits defined by a "Compute noise On" event and a 'Compute noise Off' event. Inside these limits a linear regression is calculated for the signal. The result is a y=ax+b equation. This regression straight line is subtracted to the signal and the difference between the min and max value of the 'horizontal' signal is calculated. This is then the noise. This variable can be used for blank chromatograms (no peak) during the whole chromatogram.

- **Noise Sdev [NOISE_SDEV]:** Standard deviation of the chromatogram noise. This variable is calculated over the totality of the chromatogram during the integration phase. This variable has no analytical meaning; it is only used for an internal calculation.
- **Number of missing peaks [NBMISSINGPEAKS]:** The number of missing peaks (i.e., peaks present in the peak identification table but not detected).
- **Number of Peaks [NPEAKS]:** The number of integrated peaks.
- **#Points [NPOINTS]:** The total number of the acquired points in the chromatogram.
- **Operator name [OPERATOR]:** The name of the user that performed the acquisition.
- Processing date [PROCESSDATE]: The last processing date.
- **Project name [PROJECTNAME]:** The name of the project in which the acquisition was performed.
- **Report name [REPORTNAME]:** The file name of the report style used to print the chromatogram.
- **Reprocessing list count [BATCHCOUNT]:** The total number of chromatograms in the reprocessing list, if the current chromatogram was reprocessed inside a reprocessing list. If not, the value of the variable is –1.
- **Reprocessing list name [BATCHNAME]:** The name of the reprocessing list of the chromatogram, if it was processed inside a reprocessing list.
- **Reprocessing list position [BATCHPOS]:** The position of the chromatogram in the reprocessing list, if it was created inside a reprocessing list. If not, the value of the variable is -1.
- **Reason for stop sequence [SEQSTOPREASON]:** The reason why the sequence is stopped. If several suitability tests have failed, only one of them is mentioned. This variable is computed at the end of the processing and should not be used in formulae.
- **RMS noise [RMSNOISE]:** To calculate this variable the y=ax+b equation which is in the noise calculation is used, the regression is also subtracted from the signal and then, for each slice of the 'horizontal' signal:

$$\text{RMS\_Noise} = \sqrt{\frac{\sum_{i=1}^{k} signal^2}{k}}$$

- Where k is the number of points.
- The Noise ON and OFF events have to be defined in the integration part of the method to calculate this variable.
- **Run name [RUNNAME]:** The original name of the chromatogram, entered when preparing the acquisition: prefix + Run ID.
- **Sequence count [SEQCOUNT]:** The total number of chromatograms in the sequence, if the current chromatogram was created inside a sequence. If not, the value of the variable is –1.
- **Sequence name [SEQNAME]:** The name of the sequence of the chromatogram, if it was processed inside a sequence.
- **Sequence position [SEQPOS]:** The position of the chromatogram in the sequence, if it was created inside a sequence. If not, the value of the variable is -1.
- **Software current name [SOFTCURNAME]:** The name of the software which has been used to reprocess the selected chromatogram.
- **Software current version: [SOFTCURVERSION]:** The version of the software which has been used to reprocess the selected chromatogram.

- **Software name [SOFTNAME]:** The name of the software that originally created the selected chromatogram.
- **Software version: [SOFTVERSION]:** The version of the software that originally created the data file.
- **Stop sequence [SEQSTOP]:** This variable equals TRUE if the sequence must be stopped after this chromatogram acquisition (due to a suitability test failure) and FALSE else. This variable is computed at the end of the processing and should not be used in formulae.
- **System name [SYSTEMNAME]:** The name of the system used to acquire the chromatogram.
- **Total peak area [TOTAL_AREA]:** The sum of the areas of all peaks in the chromatogram.
- **Total peak height [TOTAL_HEIGHT]:** The sum of the heights of all peaks in the chromatogram.
- **Total peak response [TOTAL_RESPONSE]:** The sum of the responses of all peaks in the chromatogram. The response is Area, Height, Area % or height%, Area $^{1/2}$ or height$^{1/2}$ according to what has been defined in the calibration method.
- **User name [USERNAME]:** The name of the user that performed the last processing.

Input Variables

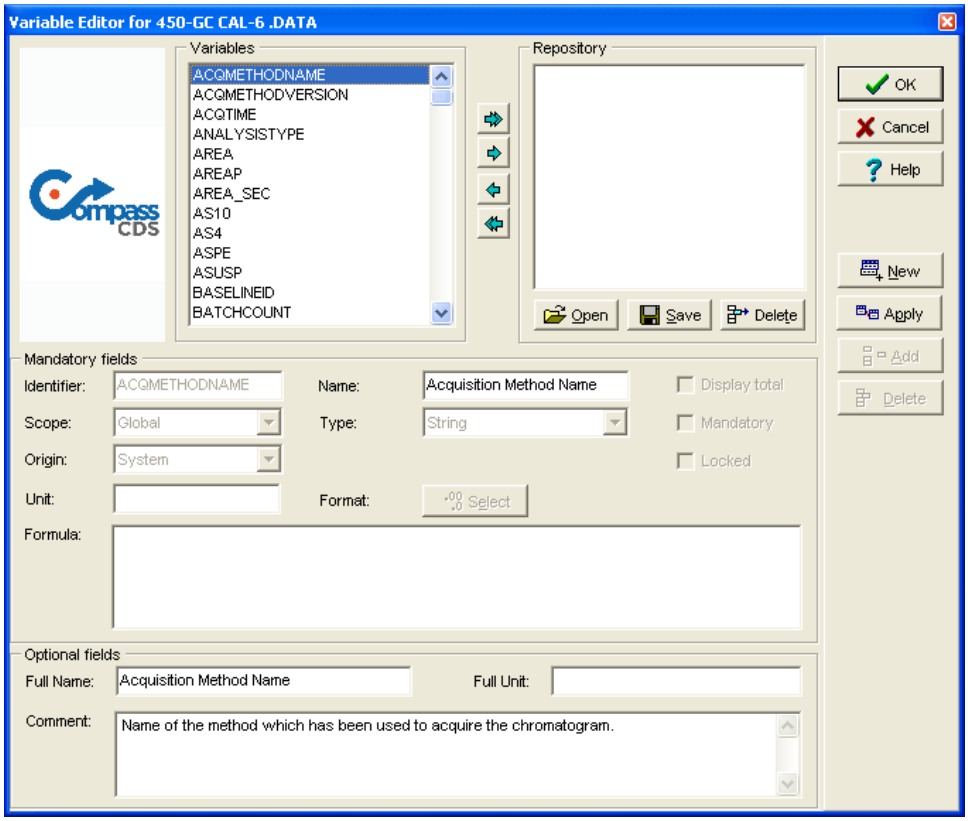
- **Dead time [DEADTIME]:** It is the dead time, entered manually at the acquisition time. It can be modified in the CHROMATOGRAM PROPERTIES after the acquisition.
- **DT [DELTAT]:** The acquisition period. It is the time between two acquisition points. This time can be changed via the Acquisition rate in the acquisition method. Deltat is the inverse of acquisition rate.
- **Divisor Factor [DIVFACTOR]:** This variable is used to divide all the quantities by a factor. This value is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **InjVoL [IVOL]:** This is the volume injected by the autosampler (if present) and if it is driven. It also can be entered for information purposes only. This value is entered when preparing the acquisition. Note that for some liquid chromatographs which injector is chosen, it can be a syringe fraction and not a volume.
- **Istd Weight [ISTDW]:** This is the internal standard quantity, if there is only one. This value is entered when preparing the acquisition and can be modified in CHROMATOGRAM PROPERTIES. When there are several internal standards, use the variable ISTDVAL ('IntStd') that gives the quantity of the internal standard named 'IntStd'.
- **Mass [MASS]:** The mass of injected sample. This value is entered when preparing the acquisition and can be modified in CHROMATOGRAM PROPERTIES.
- **Multiplier Factor [MULTFACTOR]:** This variable is used to multiply all the quantities by a factor. This value is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **#Rack [RACKNUMBER]:** It is the number of the rack used for the acquisition.
- **Run Information [RUNINFO]:** The information about the sample. This information is entered when preparing the acquisition. It can be modified in CHROMATOGRAM PROPERTIES.
- **Run Time [RUNTIME]:** It is the total acquisition time of the chromatogram.
- **#Vial [VIALNUMBER]:** The number of the vial where the sample was taken. This value is entered when preparing the acquisition to select the correct autosampler vial (if autosampler is present), or is for information purposes only.

User Input Variables

User input variables are variables created by user who has to assign a value. Two ‘user input’ variables can be defined:

- The ‘user input by peak’ (one value has to be defined by peak)
- The ‘global user input’ (one value has to be defined by chromatogram file)

NOTE: The peak or global choice is made in the “Scope” field.



For both NON MANDATORY ‘global’ and ‘by peak’ user input variables, it is possible to define a default value.

The User Input by Peak Variables

The User-Input variables are variables whose values are entered to be used for the calculation of other variables.

To create a User-Input by peak variable:

1. Add a variable in the variable editor (New button).

   Define the scope: peak.

   Define the origin as “User input”.

   Choose a short, easily remembered identifier for this variable. This identifier can be used in the formula of other custom variables if this variable is needed for other calculations.

   Define the name of the variable. The name will be used to identify the variable in the peak identification table.

Define the unit of the variable. The unit will be associated with the variable name.

Define the type and format of the variable, and optionally, add a comment for this variable.

Check the 'Mandatory' box to require the operator to enter the variable in the identification table (Identification part of the method)

Define a default value for non-mandatory variables only (optional). This option is available only if the user owns the corresponding profile in CompassCDS Configuration Manager.

The 'Lock the variable' function is available only if the user owns the corresponding profile. This option allows the user to lock a variable to forbid other users to modify it, except the format, the unit and the optional fields.

Press the Apply button.

For each peak "user input" variable, a column is added to the peak identification table in which a particular value can be defined for each peak.

Note that if the user modifies the user input default value in a chromatogram, the value is updated in the identification part of the method only for the peak that already contains the previous default value.

Example of "user input by peak" variable: Peak Purity

The analyzed sample can be composed of several compounds coming from solutions of different and known purities. To quantify those compounds, CompassCDS must take into account the purity factor of each peak (if the quantities defined in the calibration table do not take into account the purity).

2. Create a peak user input variable named PEAKPURITY. In the identification table enter the value of the purity for each component in the added column which is the variable name.

   Create a peak user formula with the formula: PEAKPURITY x QTY and display it in the peak result table.

The Global User Input Variables

The global user input variables are variables defined for a chromatogram whose values are entered when starting a single acquisition or a sequence, or in the chromatogram properties. They are entered only for information or to be used for the calculation defined by the user (user formula variable).

- In the Quick Start windows, click on the More button.
- In the sequence, select the "user input" column.
- In the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES select the Variable tab or use the icon).

NOTE: The value entered when starting an acquisition can be changed afterwards, in the chromatogram properties.

To create a new global User-Input variable:

1. Add a variable in the variable editor (New button).
2. Define the scope: global.

3. Define the origin as “User input”.
4. Choose a short, easily remembered identifier for this variable. This identifier can be used in the formula of other custom variables if this variable is needed in other calculations.
5. Define the name of the variable. The name will be used to identify the variable in the acquisition window (Quick Start or sequence) and in the chromatogram properties.
6. Define the unit of the variable. The unit will be associated with the variable name.
7. Define the type and format of the variable, and optionally, add a comment for this variable.
8. Check the ‘Mandatory’ box to require the operator to enter the variable in the chromatogram properties, the Quick start or the sequence.
9. Define a default value for non-mandatory variables only (optional). This option is available only if the user owns the corresponding profile in CompassCDS Configuration Manager.
10. The ‘Lock the variable’ option allows the user to lock a variable to forbid other users to modify it, except the format, the unit and the optional fields. This option is available only if the user owns the corresponding profile.
11. Press the ‘Apply’ button

Note that if user modifies the user input default value in a chromatogram, the value is updated in the chromatogram properties only for the variables that already contain the previous default value.

If loading a chromatogram in a reprocessing list, and then modify the default value of a global user input variable belonging to it, the user will have to load again the method to update the default value. The same behavior occurs in the sequence.

Example of a global user input variable: Sample code

Create a global user input variable called SAMPLECODE. This variable would correspond to a number or a code identifying the analyzed sample. Check the Mandatory Variable box to force the user to assign a value before each acquisition, realized either by a Quick Start or a sequence, in the corresponding field, and press Apply.

User Formula Variables

To create a new variable with specific calculations, press the NEW button. Next, specify the identifier, name and unit of the variable, then specify the scope, to determine if the variable is for the entire chromatogram (global), the groups or the peaks. Finally specify that the origin is a ‘User formula’, complete the corresponding formula (in the Formula field) and press the APPLY button.

How to Express the Formula

The formula definition must follow strict rules:

- The formula can use existing variables. To call an existing variable, use the variable identifier. (For example: AREAP for area percentage or G_RF for the response factor of a group). Enter the first variable identifier letter in the Formula field; a popup menu that lists the variables that begin with that letter is displayed. Choose the variable from the list.
- The mathematical operations of general use (addition, subtraction, multiplication, division) are defined by adding the corresponding symbol (+ - x /), for example: AREA+HEIGHT. More complicated operations are also possible, for example cosine, exponential, logarithm, etc. The corresponding syntax is detailed in the section ‘Usual Functions’, page 134.

- It is possible to define a condition. The correct syntax is:
- If (cond) then (x) else (y) is: IF (cond; x; y). The semicolon means consecutively ‘then’ and ‘else’. Conditions can overlap, so it is important to respect use of parentheses: IF (cond; IF (cond; a;b); IF (cond;x;y)).

For example, if the area of a peak is less than 150, display ‘quantity * 2’, else display “quantity * 3” is: IF (AREA<150; QTY*2; QTY*3).

The results can be real numbers, or strings. The results can also be another condition: IF ((AREA>1000); (IF HEIGHT>1000; ‘Large and high peak’; ‘Large and low peak’); (IF SKEW>=0; ‘Little tailing peak’; ‘Little fronting peak’)). In this case, the area of the peak will first be tested, then if it is larger than 1000, the height will be tested. If the peak area is less than 1000, the skew of the peak will be tested, otherwise the message 'Large and low peak appears'.

- To display text, enclose it with apostrophes; in this way CompassCDS will be able to distinguish it from a variable.
- For example, to create a variable allowing the display of the name on the chromatogram, the retention time and the area of each peak separated by a dash, define a peak variable with the formula: NAME+‘-’+RF+‘-’+ AREA. The result will be, for example, benzene-1,2-34.
- Global, group, and peak variables can be calculated with a user formula. But, if a peak variable is used in a global or a group variable formula, it is necessary to define which peak is addressed. For example if a global formula is the sum of the area of all the peaks divided by the area of the peak of Acetone: the formula will be TOTAL_AREA/AREA(‘Acetone’).The peak name must be defined between apostrophes and parentheses, with exactly the same spelling as the one defined in the identification table.

Of course, it is necessary to clearly define the group used in a global variable formula.

- The groups or the peaks can be defined by their index or by their name. Height (1) will be the height of the first peak, whereas G_QTY (‘NC12+’) will be the quantity of the group named NC12+. The name of a peak or a group is a string character. As a consequence, it is necessary to place it between two single quotes. Peak names are not case sensitive.
- A peak variable without an index or peak name will correspond to the value of the variable for the current peak. For example, the following formula AREA/AREA (‘ISTD’) will divide the area of each peak by the area of the peak named ISTD.
- In the same way, a group variable that is not identified with any index or name will be considered as the variable of the current group in a group variable.
- It is also possible to define a Boolean. A Boolean is composed of a condition expressed as a formula: *Qty (‘Benzene’) <5 or NOISE>100*. The result is True if the condition occurs or False if it is not. The condition can be composed of several conditions separated by AND, OR. Use parentheses to separate the propositions. For example (AREA<5) OR (AREA>30), if one or the other condition is accepted, the result is TRUE if no one is accepted the result is FALSE.
- To set response values other than TRUE and FALSE, use the functionality IF: IF (condition; positive result; negative result). Therefore, if the condition is true, the value of the variable will be the positive result. Otherwise, if it is false, it will be the negative result.

A Few Examples of Custom Variables

- **Annotation (peak variable):** To display the name of the peak and its retention time as the peak annotation, enter the formula NAME+ ‘ ‘ +RT. Once this variable is defined, call it from the Content zone of the peak annotations ( ).

- **Drift:** To calculate the drift between the first and the thousandth data point, the difference between the signal values at these points can be calculated. Create a global variable with the formula DATA (1000)-DATA (1). The result will be displayed in the chromatogram properties.
- Molar response percentage (by peak):

This requires the creation of three variables:

1. A peak user input whose name is MOL_RF. The corresponding values must be entered in the peak identification table for each peak.
2. A peak user formula, whose name can be INTERM, that will be used as an intermediary variable and defined by the formula: AREA *MOL_RF and calculated for each peak.
3. A peak user formula, which is the molar percentage of each peak, defined by the following formula: INTERM/SUM (‘INTERM’)*100. The user will just have to display this variable in the peak result table to know the molar percentage of each peak.

Name of the internal standard associated to each peak:

Three peak user formula variables must be created:

- ISTDINDEX (integer) : ISTD(NAME)
- ISTDNAM (string): NAME(ISTDINDEX)
- ASSOCISTDNAME (string): IF(PEAKID=ISTDINDEX;’ ‘;ISTDNAM)

Display the ASSOCISTDNAME variable in the peak result table. The internal standards will be assigned an empty value; the no internal standard one will be assigned the name of the associated internal standard.

- Name of peaks that are internal standard

In this case only one internal standard is defined; create the following peak user formula:

IF (NAME=ISTDNAME (1);'ISTD';' ')

The value of the variable will be ISTD for the peak that is internal standard and nothing for the non ISTD compounds.

In the case two internal standards are defined, create the following peak user formula:

IF ((NAME=ISTDNAME (1)) OR (NAME=ISTDNAME (2));'ISTD' ;')'

The value of the variable will be ISTD for the peak that are internal standards and nothing for the non ISTD compounds.

- Calculation of the capacity factor according a non fixed dead time value.

Two variables must be defined; one to impose the dead time equal to the retention time of the first integrated peak, the second one to calculate the capacity factor according to the value of the calculated dead time:

1. A global user formula variable, whose name is EXPDEADTIME (experimental dead time) (real) defined by the formula: RT(1)
2. A peak user formula, whose name is CAPACITY(capacity factor) (real) defined by the formula: (RT- EXPDEADTIME)/ EXPDEADTIME

- **Noise:** To calculate the noise between 1 and 2 minutes, the difference between the signal maximum and minimum can be calculated. Create a global variable with the formula 'DATAMAX (1.0; 2.0) - DATAMIN (1.0; 2.0)'. The result will be displayed in the chromatogram properties. Note that the standard system variable Noise_SDEV calculates an estimation of channel noise standard deviation.
- **Relative area (group variable):** To divide the area of each group by the area of the peak named Butadiene, the corresponding formula is 'G_AREA/AREA ('Butadiene')'. Once this variable is defined, it is possible to display it in the group report.
- **Peak validity 1:** To check that the quantity is between 10 and 20 for each peak, create a peak variable with the following formula: IF ((QTY>=10) AND (QTY <=20); 'OK'; 'not OK'). If this variable is selected in the peak report, a new column will appear, stating OK if the quantity of the peak is between 10 and 20 or alternatively not OK if the quantity is not between 10 and 20.
- **Peak validity 2:** There is another way of processing to obtain a similar result. Define a Boolean with the formula (QTY>=10) AND (QTY <=20). The result will be either 'True' or 'False'.
- **Prefix:** To display the RUNNAME without the RUN ID. Create a global user formula, with the following formula: COPY (RUNNAME; 1; POS ('-'; RUNNAME)-1).
- **Relative Response Factor (peak variable):** To divide the response factor of each peak by the response factor of a defined peak, the corresponding formula is 'RF/RF (name of reference peak)'. The first possibility is to type the name of the peak instead of 'name of reference peak' in the formula, the second possibility is to create a global variable (for example 'RefName'), which is a user input and mandatory. The formula should be changed into 'RF/RF (RefName)'. Before acquisition, the user will enter manually the name of the reference (a default value can be entered for the method), and all the response factors of the peaks will be divided by the response factor of the compound whose name will be specified in the acquisition window.
- **Relative Quantity:** To calculate the difference between the quantity of a peak and the quantity of the previous peak, divide it by the height of the next peak. Define a peak variable with the following formula: (QTY-QTY (PEAKID-1))/HEIGHT (PEAKID+1).
- To calculate the area of the 10th peak plus the area of the peak named 'Benzene' and divide the result by the sample weight. Create a global variable with the following formula: (AREA (10) +AREA ('Benzene'))/ SMPWT. The corresponding variable will be displayed in the chromatogram properties.
- How to print only a part of a variable value. For example the name of chromatogram is 'test-1', and you want to print only 'test'. Create a global variable with the following formula: COPY (CHROMATONAME; 1; POS ('-'; CHROMATONAME)-1).

Usual Functions

The list of the usual functions proposed by CompassCDS is detailed in this part of the manual, as the syntax to respect (parenthesis, cots, etc.)

In the following paragraph, X represents the identifier of the variable on which the calculation is performed.

- **ABS(X):** The result of this function is the absolute value of the parameter. For example: ABS (SKEW)).
- **ARCTAN(X):** The result of this function is the arctangent of the parameter.
- **BOOLEAN:** This function transforms the character strings 'TRUE' and 'FALSE' into the Boolean values TRUE and FALSE.

- **CALCOEFF (‘compound name’; ‘coefficient’):** The result of this function is the value of the specified coefficient in the calibration table of the compound defined in the parameters. For example, CALCOEFF (‘Benzene’;’ a') gives the value of the coefficient of the benzene calibration curve.
- **CALCOEFF ('compound name '; ‘COR’):** Using the previous function, enter the special coefficient ‘COR’, and the result will be the regression coefficient of the specified compound curve.

For example, CALCOEFF (‘Benzene’;’ OR')

- **COPY(X; Y; Z):** The result of this function is a part of a variable value. X represents the variable name, Y the position of the first character to copy, Z the position of the last character to copy. For example the chromatogram name is ‘first-quality-test’, and you want to display ‘quality’, the variable to create is: COPY (CHROMATONAME;7;13), where 7 corresponds to the position of the ‘q’ and 13 to the position of the ‘y’ in the entire chromatogram name.
- **COS(X):** The result of this function is the cosine of the parameter.
- **CSUM (‘X’):** The result of this function is a real number, and is the cumulative sum of the variable for the peaks or groups (depends if it is a peak or a group variable). The variable to be summed should be a real number. For example, if the areas of the three peaks of a chromatogram are 10,000; 50,000 and 20,000, then CSUM (‘AREA’) equals 10,000 for the first peak, 60,000 for the second peak, and 80,000 for the last peak.
- **DATA (integer) or DATA (real):** The result of this function is a real number, and is the value of the signal for the slice or the retention time that is given as the parameter. If the parameter is a real, the value of the signal at the corresponding retention time will be given. However, if the parameter is an integer, the value of the signal at the corresponding slice number will be given. Data (10) will be the signal value of the 10th slice, while Data (10.0) will be the signal value at the 10th minute.
- **DATAMAX (integer; integer) or DATAMAX (real; real):** The result of this function is a real number, and is the maximum value of the signal between the two slices (if arguments are integer) or between two times (if arguments are real). The corresponding slices or times are defined as parameters.
- **DATAMIN (integer; integer) or DATAMIN (real; real):** The result of this function is a real number, and is the minimum value of the signal between two slices (if arguments are integer) or between two times (if arguments are real).The corresponding slices or times are defined as parameters. Datamin (0, 1000) will be the minimum value of the signal between the first and the 1000th slices. Datamin (8.2, 8.5) will be the minimum value of the signal between 8.2 and 8.5 min.
- **Date:** This function provides the current date. The result of this function is a string. For example, the value of this function could be ‘10/07/99’.
- **DAYSBETWEEN:** This function is useful to calculate the number of days between two dates. DAYSBETWEEN (a; b) compares the number of days between a and b. The result is an integer. For example
- DAYSBETWEEN ('01/12/99'; ACQTIME),
- DAYSBETWEEN ('today'; CALDATE),
- DAYSBETWEEN ('December 12, 1999';'january 1, 1998'),
- DAYSBETWEEN ('today';'monday').
- The character strings describing the dates will follow the regional settings for Windows.
- **EXP(X):** The result of this function is the exponential of the parameter.

- **FLOAT(X):** This function is the inverse of string: it transforms the parameter (integer or Boolean) into a real number if possible. In the case of a Boolean value, TRUE is transformed into 1.00 and FALSE is transformed into 0.00.
- **FRAC(X):** The result of this function is the decimal part of the parameter. For example, FRAC (11.258) is 0.258.
- **GROUPID:** This function is useful for group variables. It provides the index of the group for which the variable value is calculated. For example, AREA (GROUPID)/AREA (GROUPID-1) will be used to calculate the ratio of the area of the current group to the area of the previous group.
- **INT(X):** The result of this function is the whole number part of the parameter. For example, INT(11.258) is 11.0. The result is a real number, whereas the result of TRUNC is an integer.
- **ISTD ('compound name') or ISTD (NAME):** The result of this function is the index of the internal standard associated with the peak or the group set as a parameter. If a peak variable is created with the formula 'ISTD (NAME)', the index of the internal standard associated with each peak in the peak table will be displayed.
- **ISTDNAME (I):** The result of this function is the name of the ith internal standard (in the order of appearance in the chromatogram properties).
- **ISTDVAL ('IntStd'):** The result of this function is the quantity entered for the internal standard which name is 'IntStd'.
- **LENGTH(X) or LENGTH ('text'):** This function gives the number of characters in the string set as a parameter. For example, LENGTH ('STRING')=6.
- **LN(X):** The result of this function is the natural logarithm of the parameter.
- **LOWER(X) or LOWER ('text'):** This function transforms the character strings into lower case. For example, LOWER ('STRING') ='string'.
- **MAX ('X') or MAX ('X'; n):** This function calculates the maximum value of the peak or group variable defined as a parameter. This function can also be used to calculate the nth maximum value. For example, MAX ('HEIGHT';2) is the second maximum height.
- **MAXID ('X') or MAXID ('X'; n):** This function calculates the index of the peak (or group) which has the maximum value for the variable defined as a parameter. This function can also be used to calculate the index of the peak or group that has the nth maximum value.
- **MIN ('X') or MIN ('X'; n)::** This function calculates the minimum value of the peak or group variable defined as a parameter: MIN('AREA') is the minimum area of the peaks. This function can also be used to calculate the nth minimum value: MIN ('G_AREA'; 2) is the 2nd smallest group area.
- **MINID ('X') or MINID ('X'; n)::** This function calculates the index of the peak (or group) which has the minimum value for the variable defined as a parameter: MINID('AREA') is the index of the smallest peak. This function can also be used to calculate the index of the nth minimum value: MINID ('G_AREA'; 2) is the index of the 2nd smallest peak.
- **PEAKID:** This function is useful for peak variables. It provides the index of the peak for which the variable value is calculated. For example, AREA (PEAKID)/AREA (PEAKID-1) will be used to calculate the ratio of the area of the current peak to the area of the previous peak.
- **PI:** is the constant π.
- **POS(X;Y):** This function gives the position of a character (or a group of characters) in a variable. For example you want to know the position of 'quality' in the chromatogram name 'first-quality-test'. The variable to create is POS ('quality'; CHROMATONAME), the result is 7, corresponding to the position of the q in the chromatogram name.

- **POWER (a; b):** This is a two-parameter function: POWER (a; b) is equal to “a” to the power of “b”.
- **REALEQUAL (a; b; c):** This function is used to compare two real numbers. The result of REALEQUAL (a; b; epsilon) is TRUE if “a” equals “b” within the tolerance epsilon, e.g. REALEQUAL (HEIGHT; 10,000; 10) will be true if the height is between 9,990 and 10,010.
- **ROUND(X):** This function is used to transform a real number into an integer by rounding it to the closest integer. ROUND (11.8) is 12 and ROUND (11.49) is 11.
- **SIN(X):** The result of this function is the sine of the parameter.
- **SQR(X):** The result of this function is the square of the parameter.
- **SQRT(X):** The result of this function is the square root of the parameter.
- **STRING(X):** This function transforms the parameter (a real number) into a character string: STRING (1.23) is ‘1.23’.
- **SUM (‘X’):** The result of this function is a real number and is the sum of the variable for all the peaks or groups (depending if it is a peak or a group variable). The variables to be summed should be real numbers. For example, SUM (‘AREA’) equals the variable TOTAL_AREA and is the sum of the areas of all the chromatogram peaks.
- **Time:** This function provides the current time. The result of this function is a string. For example, the value of this function could be ‘15:22:30’.
- **TRUNC(X):** This function is used to transform a real number into an integer by deleting the decimal part of the number. Example: TRUNC (11.8) is 11.
- **UPPER(X) or UPPER (‘text’):** This function transforms the character strings into upper case. For example, UPPER (‘String’) =’STRING’.
- **+:** This function is useful to attach several character strings: ‘Date: ’+Date equals ‘Date: 6/16/99’. The result of an attachment with a character string will always be a character string.

Variable Repository

The variables are associated with a method. If a variable is defined in a method, and is needed for use in another method, the variable can be stored in the repository:

Define the variables needed in the first method.

In the variable editor, click and drag them to the repository, or move them with the arrows (and). It is possible to remove some variables from the repository using the Delete button.

Save the repository using the Save button.

In the other method, open the repository using the Open button.

Import the variables needed using the button.

It is possible to use the repository to move the changes that were made on the standard variables (name, format…). Save the corresponding variables in the repository, open it in the method, and then import them as different variables.

A repository named ‘Additional variables.REPO’ is available. It contains the following peak variables.

AS13: peak asymmetry (half width at 13,4%).

AS32: peak asymmetry (half width at 32,4%).

AS50: peak asymmetry (half width at 50%).

AS60: peak asymmetry (half width at 60.7%).

FLAG1: If the peak is saturated (value of the ISSAT variable = TRUE), then the variable has the value ‘Saturated’.

FLAG2: If the height of the peak is inferior to the value of the LOQ variable (limit of quantification), then the variable has the value ‘Below LOQ’. Do not forget to add the LOQ variable in the variable list.

FLAG3: If the start or stop peak markers have been defined manually, the variable has the value ‘Manual integration’.

FLAG4: If the height of the peak is inferior to the value of the LOD variable (limit of detection), then the variable has the value ‘Below LOD). Do not forget to add the LOD variable in the variable list.

LOD: Limit of detection, the variable equals to NOISE*3 (do not forget to add the COMPUTE NOISE ON and OFF integration events in the integration table).

LOQ: Limit of quantification, the variable equals to NOISE*5 (do not forget do add the COMPUTE NOISE ON and OFF integration events in the integration table).

PEAK SIGN: If the ISPOS variable value is ‘TRUE’, ‘the variable has the value ‘positive’ and ‘negative’ if not.

P_ANNOTATION: If the peak is identified, the variable value is the name of the peak. If it is an unknown the variable value is its retention time.

P_ANNO_NAME_QTY: The variable value is the name of the peak plus its quantity plus its unit. Do not forget to edit the variable and replace the word ‘unit’ by the correct unit in the formula field.

P_ANNO_NAME_RF: The variable value is the name of the peak plus its response factor.

P_ANNO_NAME_RT: The variable value is the name of the peak plus its retention time.

P_ANNO_RT_NAME: The variable value is the retention time of the peak plus its name.

P_ANNO_RT_NAME_AREAP: The variable value is the retention time of the peak plus its name plus its area percent.

P_ANNO_RT_NAME_CODE: The variable value is the retention time of the peak plus its name plus its code (see the CODE variable definition).

P_ANNO_RT_PGROUP: The variable value is the retention time of the peak plus the name of the group it belongs to, if any.

The ‘Additional variables REPO’ file is stored in the COMPASSCDS / SERVER / DATA SHARED directory.

RF_SEC: The variable value is the response factor expressed in Qty unit/µV.sec. It corresponds to the calculation RF*60.

NOTE: For all the annotation variables, do not forget to check the ‘annotate unknown peaks’ option in the peak annotation screen and to select the P_ANNOTATION variable in the Content field.

Baseline Monitoring / Quick Start / Sequence

The baseline monitoring allows the signal generated by the system to be viewed, without the need of any injection. Quick Start and Sequence allows injection of one or several samples. During a baseline monitoring, no data file is generated whereas during an acquisition (Quick Start or sequence) data files are generated.

Before starting a baseline monitoring or an acquisition, a method must be prepared for the corresponding system (chromatograph).

Baseline Monitoring

To monitor the baseline before starting an acquisition, select the menu ACQUISITION / MONITORING BASELINE.

A window appears in which it is possible to select which system should be monitored. (When logged in with the 'All projects' mode, the project must first be selected). Now choose the method to be used to condition the apparatus: the initial parameters of the method are sent to the system so that it is prepared for the analysis.

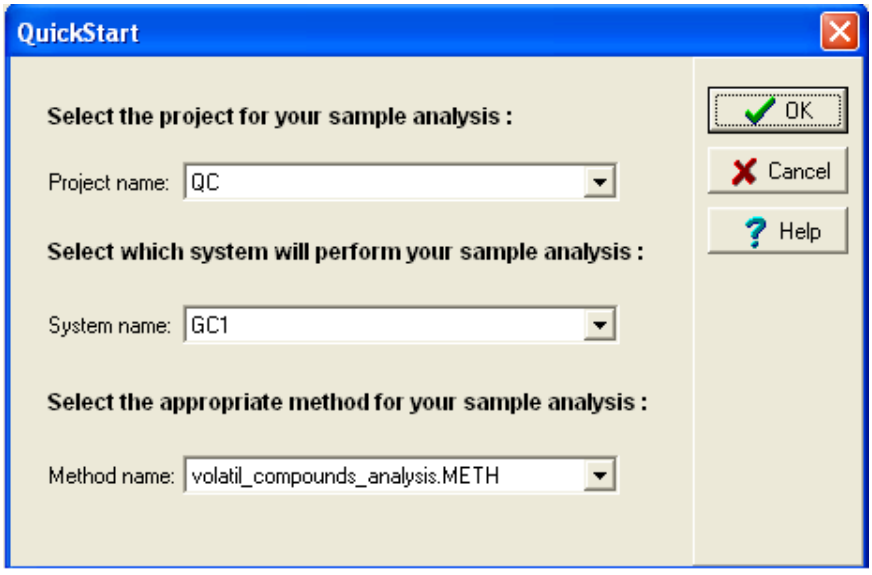
The signal is then displayed in the acquisition window (system tab) as for normal acquisitions. When the system is ready, press the 'stop' button to cancel monitoring and allow the start of an acquisition.

Quick Start

Single Acquisition

To start a single acquisition, select the menu ACQUISITION / QUICK START or press the corresponding icon .

The following window appears:



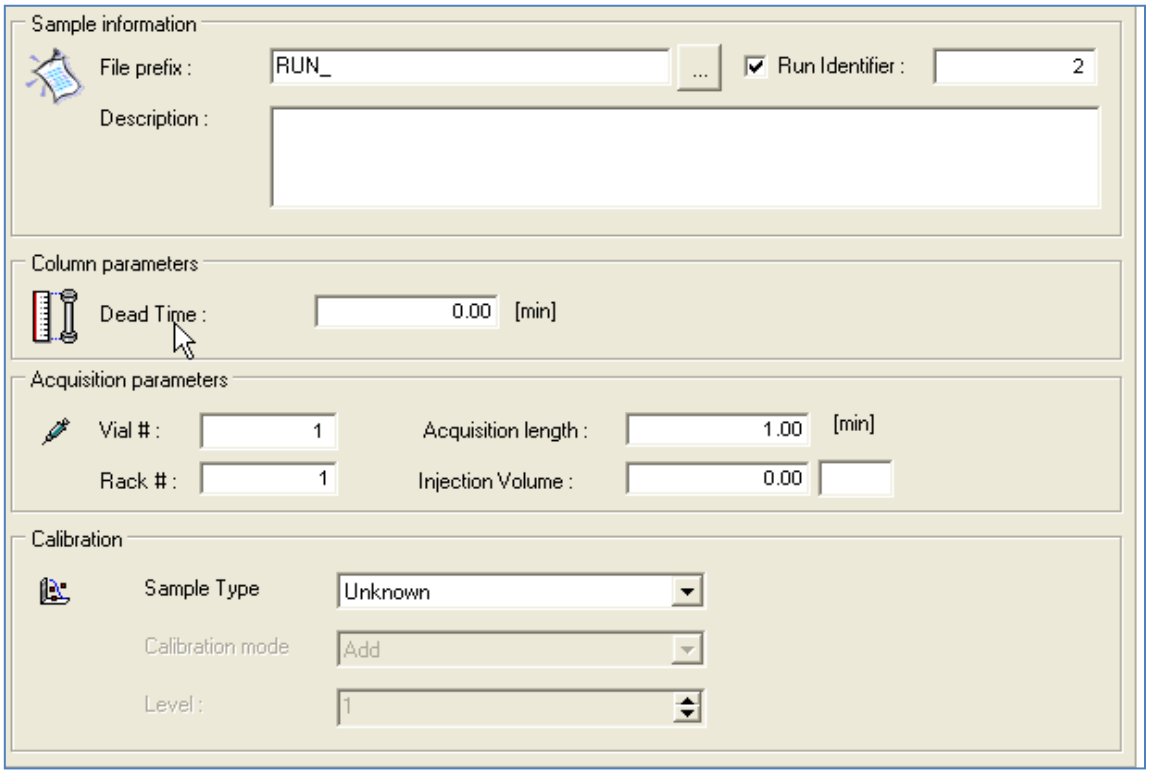
In this window, select the project associated with the acquisition (if connected in all projects). The chromatogram will be stored with the files associated with this project.

Next, select the system (chromatograph) for sample injection. CompassCDS will only display the system names that are associated with the specified project.

Now select the method that will be used to acquire and process the sample. CompassCDS will only display the method names that are associated with the specified system.

Press OK.

The Quick Start window now appears. The default acquisition parameters set in the method are displayed in this window.



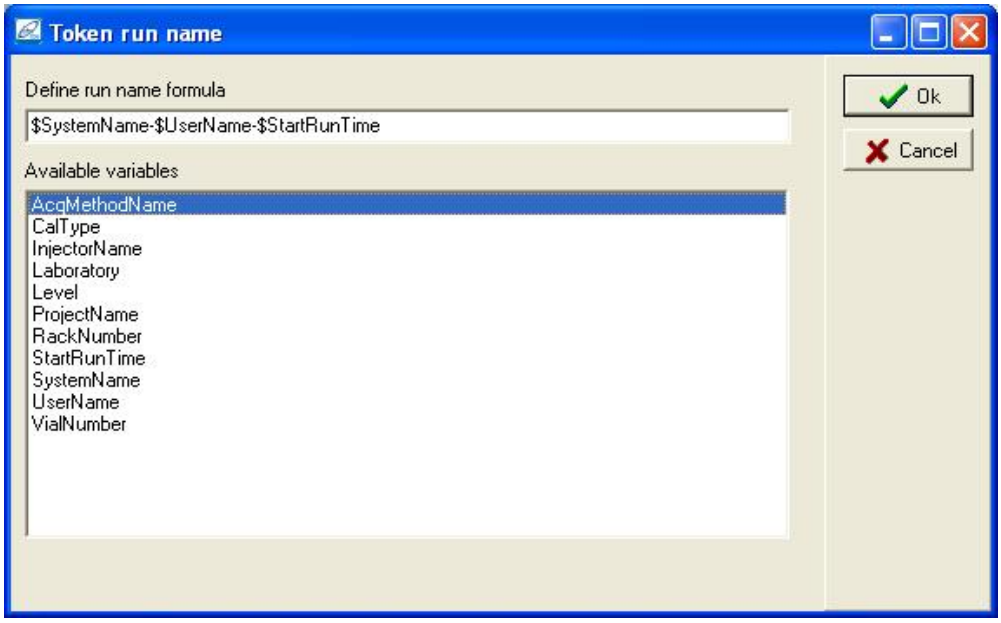
In the Acquisition parameters tab, define all the parameters common to all channels.

The name of the project, system and method just selected are automatically displayed at the top of the window.

In the sample information section, enter:

File prefix: This specified the first part of the chromatogram name. The chromatogram name will be completed with the identifier. The prefix should not contain \ /:*?"<>|.

The prefix can be generated automatically by the software according to variables values. To define the ‘Token run name’, click on the ... button, and compose the token by selecting the variables (double click) in the list:



Run identifier: The second part of the chromatogram name is specified here. The index is automatically incremented in the case of the Quick start.

For example, if the file prefix is 'Run_', and the identifier is 55, the name of the chromatogram will be Run_55.data.

It is also possible to deactivate the Run identifier addition, by unchecking the associated combo box.

NOTE: If the user is not assigned the permission to overwrite chromatogram, and that a chromatogram with the same name as the one defined in the Quick Start screen already exists in the logon path, no message will appear to inform the user, and the generated chromatogram name will be the user defined name plus the acquisition date and time. The existing chromatogram will not be overwritten.

If the user is assigned the permission to overwrite chromatograms, no message will inform him that a chromatogram with same name exists, the chromatogram will be overwritten.

Description: User can enter a description that may be printed in the report.

In the column parameters section, enter the dead time (min)

In the acquisition parameters section, enter:

The vial number (alpha numeric value can be entered according to the sampler type).

The Rack number.

The Injection volume.

The Run Time (total length of the acquisition).

In the Calibration section, enter:

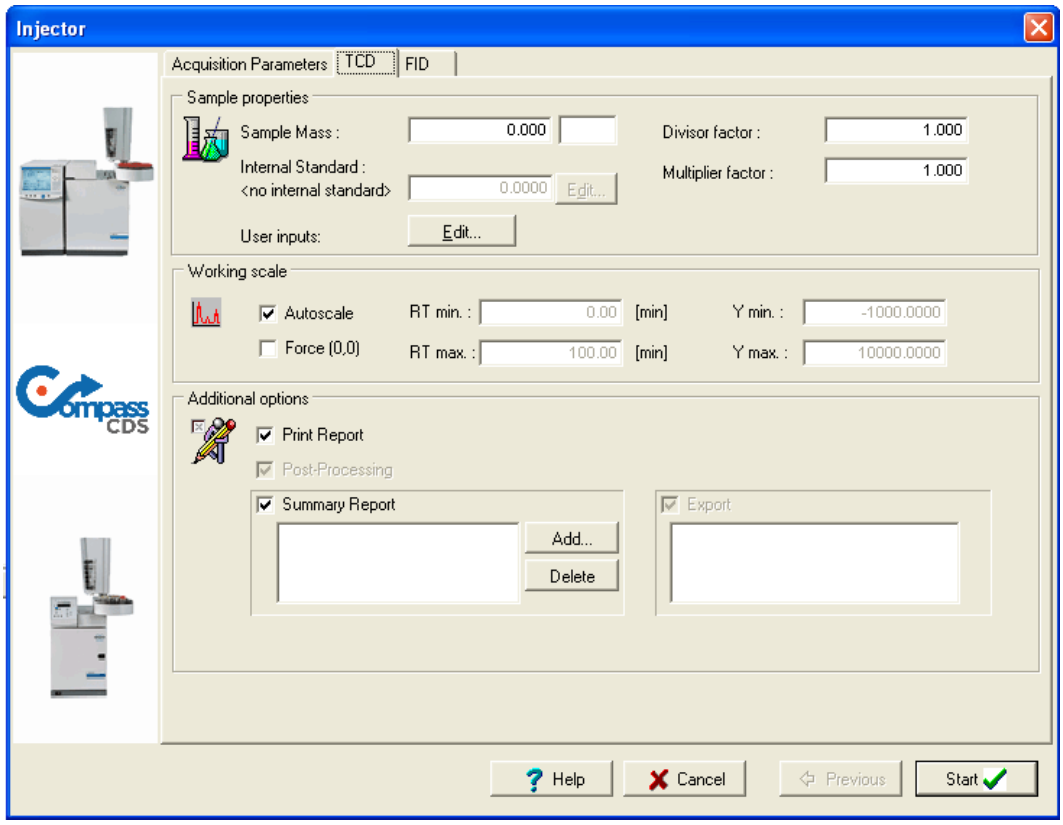
Sample Type: Define whether the chromatogram is a blank, an unknown, a standard, a control sample or a control sample (level I). According to the option selected, the chromatogram process is different.

Calibration mode: This option is available if the user is assigned the right to overwrite calibration curve. It allows the user to delete the existing curve and to build a new one by selecting 'Clear old points', or erase only the points of the defined level by selecting 'Clear level only', or add the calibration point to an existing curve by selecting 'Add'.

Level: This option allows the user to define the level in case of 'Standard or Control Sample (level I) sample' type selection.

NOTE: If the sample type is 'Control sample (level I)', and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level I) in case of suitability test failure.

Select the Channel X tab, to enter the parameters channel by channel. The following screen is displayed:



If a multi channel system is used, CompassCDS offers the possibility to define identical values for all channels (by default) or to enter channel specific parameters if the corresponding option is defined in the chosen method (refer to the 'Acquisition' part of 'The Method' section, page 34). If this option is not defined, the user defines the sample properties and the Working scale only in one tab; the other channel tabs are automatically duplicated.

In the sample properties section, enter:

Sample Mass: The mass of the injected sample

Istd: Internal standard quantity(ies), if defined in the calibration part of the method.

M: Multiplier factor

D: Divisor factor

Global User Input: global variables defined by user.

In the **Working scale** section:

Auto scale: If this option is checked, CompassCDS adjusts the chromatogram Y scale according to the max height signal. If not checked, the user specifies the X and Y limits in the corresponding fields. These limits will be the full scale in the acquisition view (System tab) and in CompassCDS main screen (Data tab) when opening the chromatogram. It is possible to modify the scale of the chromatogram after its acquisition, by pressing the icon (see page 181).

NOTE: If only the part of the signal corresponding to the working scale is displayed on the screen, remember that all points of the chromatogram are stored in the data file and potentially displayable.

Force (0, 0): Forces the acquisition view to display the origin point. This function does not force the signal to pass through the origin.

In the **Processing options** section, specify which parts of the process have to be executed by checking them.

When all the parameters have been defined, press the start button

. The control parameters are transmitted to the system and the acquisition starts immediately or when the CompassCDS Chromatography Data System receives the automatic or manual start.

Note that the ‘Quick Start’ screen is almost the same as the acquisition part of the method one. The format (number of significant digit, scientific format) of some options of the ‘Quick Start’ is customizable in the acquisition screen of the associated method, but NOT modifiable from the ‘Quick Start’ screen. The customized variable formats are:

In the ‘Sample Properties’ part: every variable

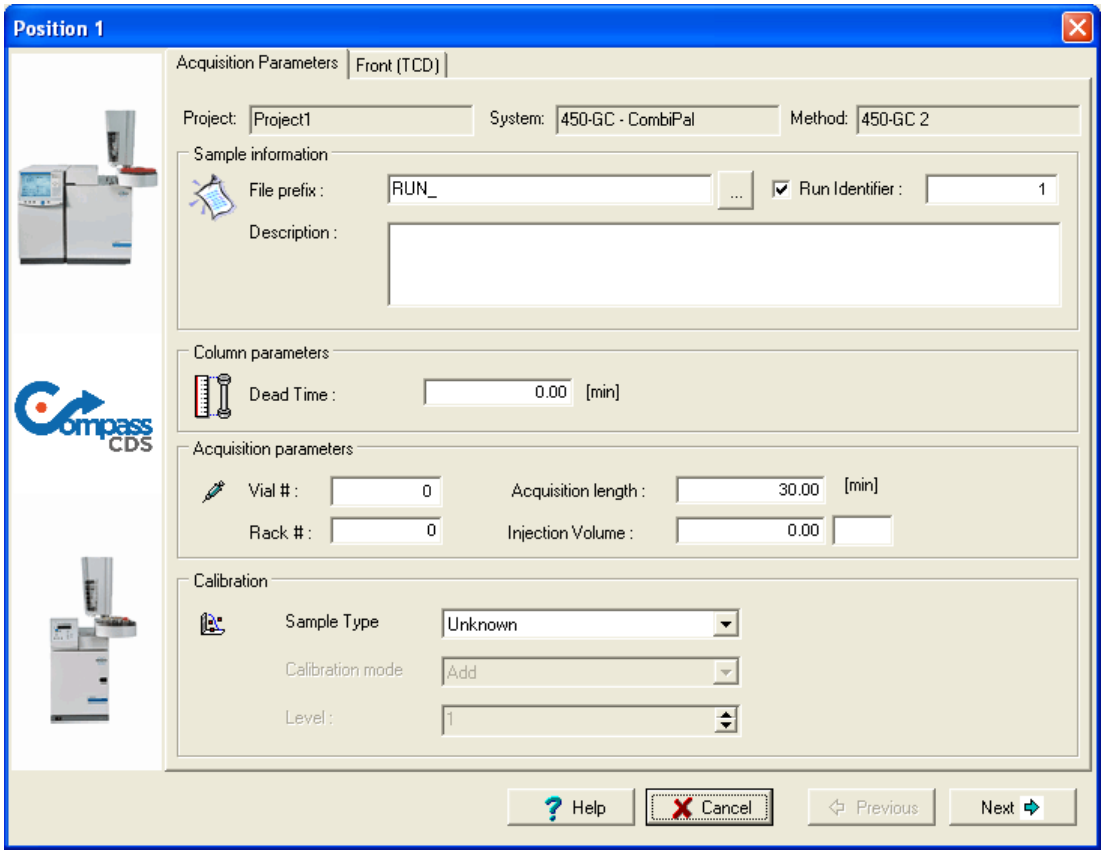
In the ‘Column parameters’ part: the Dead time

In the ‘Acquisition parameters’ part: the Run time

In the ‘Working scale’ part: RT min and RT max

In the case of multi injector systems, the Quick Start function starts as many acquisitions as injectors. As several chromatograms are created (one for each injector), several acquisition windows are completed. Each injector gives its name to the corresponding acquisition window.

Once project, system and method have been selected, the following screen is displayed:

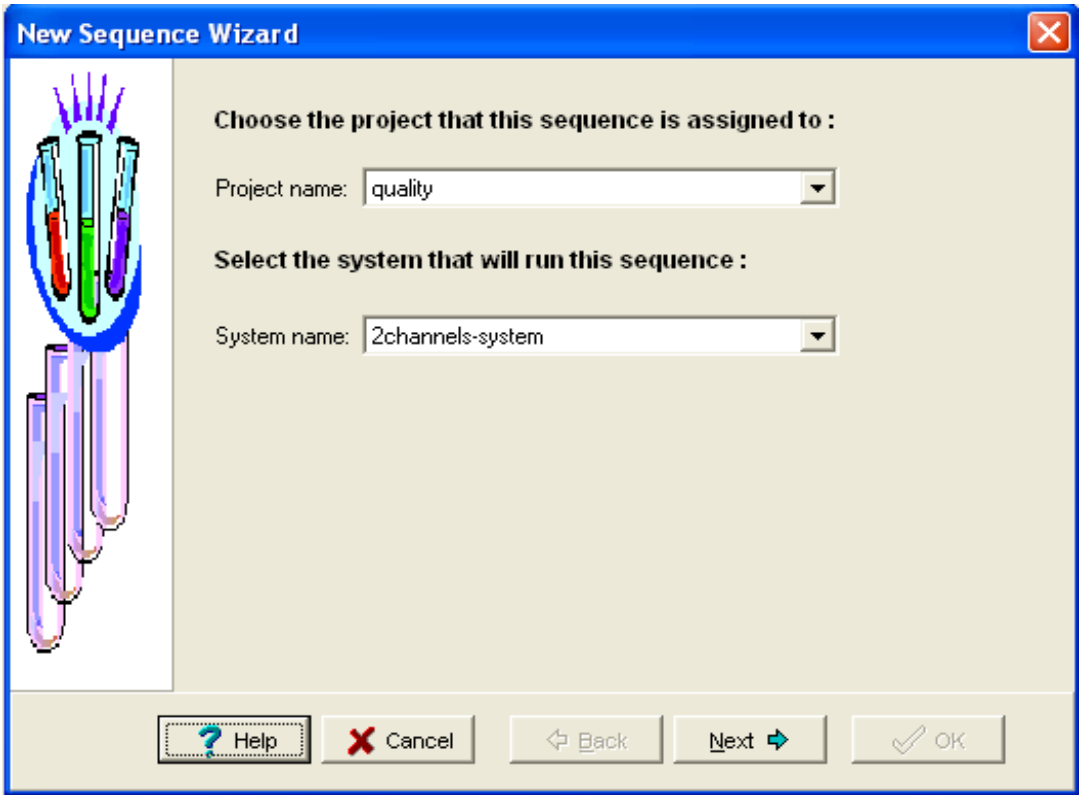


In the first injector acquisition window, the ‘Next’ button allows the access to the second injector parameters, and so on, according to the injector number defined. To come back to the previous injector screens, click on the ‘previous’ button. Once all screens are configured, click onto the ‘Start’ button to launch all acquisitions.

Sequence

To create a sequence: Select the menu options FILE / NEW / NEW SEQUENCE**.**

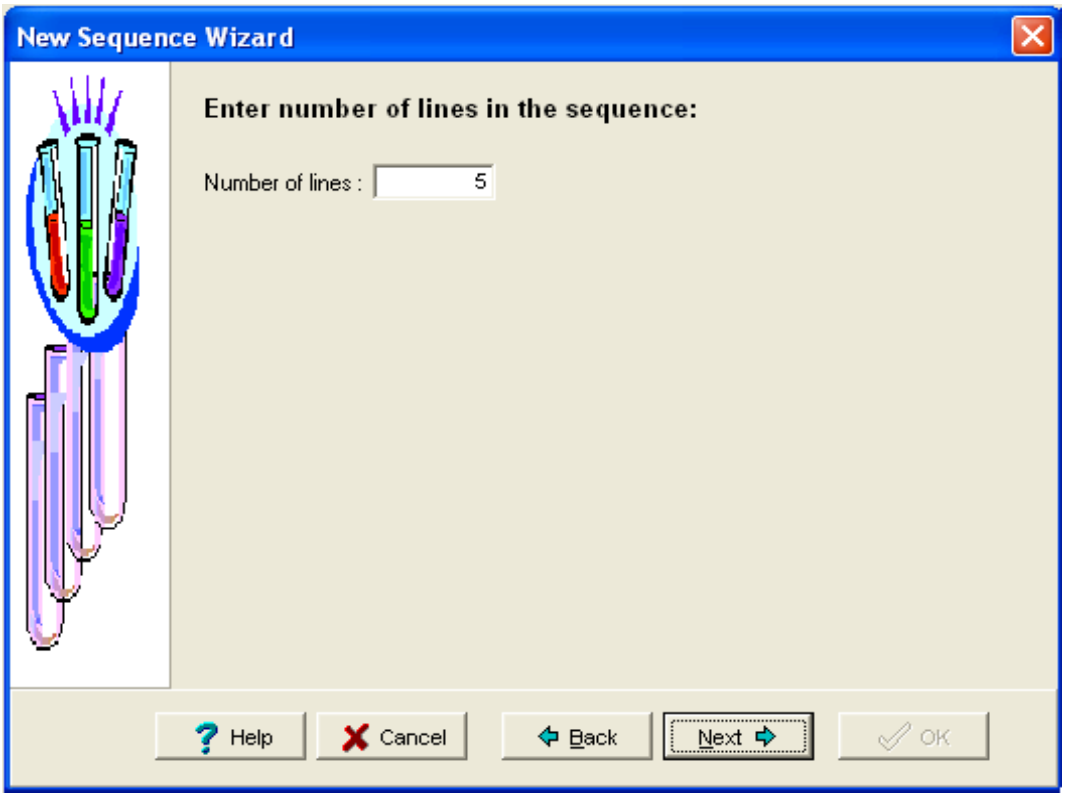
A wizard guide is available for the first steps of the sequence creation:



In this window, select the project associated with the acquisitions (if connected in all projects). The chromatograms will be stored with the files associated with this project.

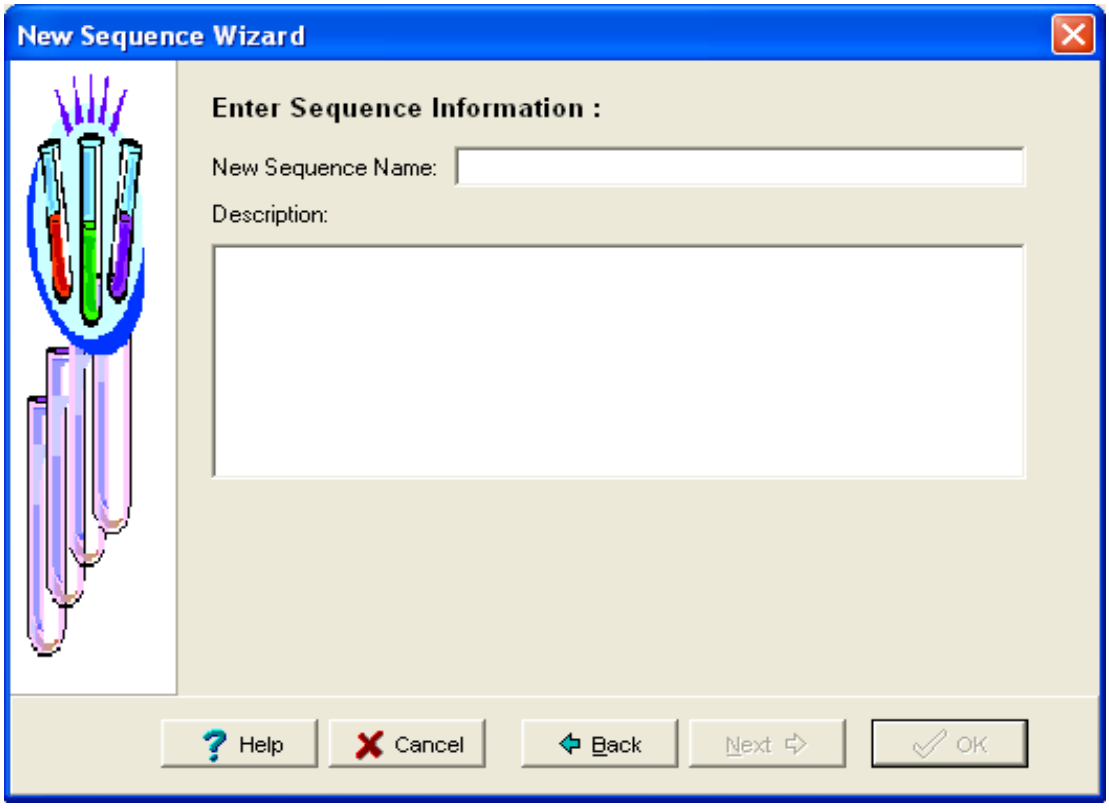
Next, select the system for sample injection. CompassCDS will only display the system names associated with the specified project.

The Next button is now active, and the second step of the method creation can be accessed to specify the number of lines in the sequence:



Each line corresponds to a sample. It is possible to add or delete sequence lines after sequence creation.

Press the NEXT button to access the third step of the sequence creation:



Enter the name of the sequence in the first edit box. In the description field, enter information about the sequence. This information will be displayed in the open file window.

The OK button is now active, after this button is pressed; the sequence is created and opened in CompassCDS.

The following sequence information is displayed at the top of the sequence graphic window:

- The name of the sequence.
- The name of the user connected / the name of the user group / the name of the project containing the sequence / the name of the system associated with the sequence.
- Near this information, the following sequence status information is also provided:

IDLE: This means that the sequence has not been launched yet or is still being created.

BEFORE RUN means that some control parameters have been sent to the system, which is about to start.

RUNNING means that a chromatogram is being acquired.

COMPLETED means that the sequence has been performed without any recorded errors.

ERROR means that a problem has occurred during acquisition. A detailed message will identify which type of error was recorded.

PAUSE AT THE END OF RUN: The sequence has been paused at the user's request, and the acquisition is still running. The user will decide at the end of the run to perform or not the rest of the sequence.

STOPPING RUN: The run is being stopped.

STOPPED: This message means that the sequence has been stopped manually.

PAUSED: This message means that the sequence has been paused manually.

SEQUENCE RESET: This message means that the sequence has been reset and can be re-launched.

CONNECTION LOST: This means that the connection has been lost. This is an abnormal state.

CONNECTION RECOVERED: This means that the connection has been lost and then recovered. No acquisition points should be lost with this type of error.

The Sequence Columns

- **No:** This is the sequence line.
- **Enabled:** This specifies whether the corresponding sequence line acquisition must be performed or not. The acquisition is performed if the box is checked.
- **Method:** In this column the name of the method to be used to acquire and process the chromatogram must be defined.
- **Method properties:** In this column it is possible to deactivate certain process of the chromatogram. Press the button and uncheck any process, which should not be executed at the end of the acquisition (e.g. export, printing, summary report or post processing).

- **Run name (prefix):** Specify the first part of the chromatogram name in this field. The chromatogram name will be completed with the identifier. This part of the name should not contain such characters as \ /:*?"<>|.
- The prefix can be generated automatically by the software according to variables values. To define the 'Token run name', click on the button, and compose the token by selecting the desired variables in the displayed screen. (See Quick Start / Single Acquisition chapter).
- **Run ID (Suffix):** Specify the second part of the chromatogram name in this field. For example, if the file prefix is 'Run_' and the identifier is 55, the name of the chromatogram will be Run_55.data. This parameter has to be an integer.
- **Description:** Information about the run may be entered in this area. This information will be saved with the chromatogram and displayed in the open file window and in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES). The description has a maximum length of 255 characters.
- **Run time:** Specify the total acquisition time in this field. The time should be greater than 0.1 and less than 1000 minutes. The sum of all the run times is displayed at the top of the sequence.
- **Injection Number:** Allows repeat injection of the same sample. The corresponding DATA files suffix will be incremented automatically: e.g. sample1_1, sample1_2.
- **Vial:** The vial number can be entered for information purposes only, or is used to specify which autosampler vial number should be injected if the instrument is controlled. According to the injector installed, alphanumeric values can be entered (refer to the injector constructor manual).
- **Rack:** The rack number is used to specify the rack number, which contains the vial with the sample to be injected if the controlled autosampler contains several racks.
- **Inj. Vol.:** The injection volume can be entered in this cell for information purposes only or can be used to specify injection volume for an autosampler, which is fully controlled by the CompassCDS Chromatography Data System.
- **Sample type:** Define, using this box, whether the injected sample is a standard, an unknown, a blank, a control sample or a control sample (level-I).
- **Calibration:** If the injected sample is a standard, choose whether the calibration point must be added to an existing calibration curve (add), or if the existing calibration curve must be overwritten (clear old points).The last possibility is to delete all the points of the defined level by choosing Clear level only.

NOTE: If the user is not assigned the right to overwrite chromatogram, and that chromatogram(s) with the same name as the one(s) defined in the sequence already exists in the logon path, no message will appear to inform the user, and the generated chromatogram name will be the user defined name plus the acquisition date and time. The existing chromatogram will not be overwritten.

In the other hand, if the user is assigned the right to overwrite chromatograms, no message will inform him that a chromatogram with same name exists, the chromatogram will be overwritten.

NOTE: If the sample type is 'Control sample (level I)', and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level I) in case of suitability test failure.

- **Level:** If the injected sample is a standard or a control sample (level-I), choose the corresponding level in this cell.
- **Istd values:** Press the button to enter the quantity (ies) of the internal standard(s).

- **User input:** In this column, it is possible to specify user input variables if some have been specified in the method.
- **Divisor:** This variable is used to divide all the quantities calculated for unknown samples by a factor. If owning the corresponding profile (to define in CompassCDS Configuration Manager) the quantity of standards will also be divided by this factor.
- **Multiplier:** This variable is used to multiply all the quantities calculated for unknown samples by a factor. If owning the corresponding profile (to define in CompassCDS Configuration Manager) the quantity of standards will also be multiplied by this factor.
- **Sample mass:** Enter the total mass of the sample in this field. This value is mandatory if the calibration mode defined in the method is mass ratio or mass%.
- **Dead time:** This time corresponds to the time required for the sample solvent (or any non-retained compound) to reach the detector. This time is used for the calculation of the selectivity and capacity factor.

NOTE: All the parameters entered in the sequence are saved with the chromatogram. Many are visible in the chromatogram properties (DATA / CHROMATOGRAM PROPERTIES) once the chromatogram has been acquired and opened in CompassCDS. The following ones can be modified in the chromatogram properties: user input variables, description, sample mass, divisor, multiplier, dead time, Internal standard values.

Use the icon to hide columns if you do not need to modify their content.

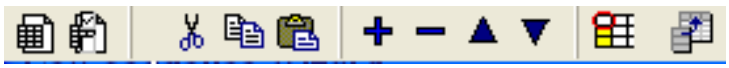
NOTE: If defining “Blank” sample(s) in the sample type column, and using a method with a chromatogram name defined in the pre-processing part, the blank subtracted will be the one defined in the type column.

Filling the Sequence

Each line corresponds to one sample.

In the first column of the sequence, select the name of the method to be used to acquire and process the chromatogram corresponding to the current line. Most of the cells in the line are filled using the values set in the acquisition part of the method, of course, these values can be modified later.

Next, fill the other columns. The sequence bar provides support tools (Most interesting is the Fill block icon):



	This icon clears the content of all the cells of the sequence.
	This icon clears the unchecked lines of the sequence.
	This icon adds a line at the end of the sequence.
	This icon deletes the selected line.
	This icon moves the selected line up.
	This icon moves the selected line down.

	This icon fills several cells of the same column according to the content of the first one. For example, to fill the 'Run ID' column, select the cells to be filled in the column, then fill the first cell with 1. Press this icon. A window appears to define the way the number will be increased. Press *OK*, and the cells are filled. If the column contains a real value or the method, the content of the first cell is simply copied, then pasted in all others.
	This icon permits selected columns to be hidden. Press this icon, and a 'Columns' window appears. Unselect the columns to hide then click on OK. Be careful not to hide cells that must be filled in before the run.

The Method properties, User input, Information and Istd values columns are filled using the button. The size of the columns can be easily modified. Place the mouse between the headers of two columns: the cursor's appearance is modified () then click on the limit between the two columns and drag it to the new position. In the same way, if you click on a column header and drag it to a new position, the column order is modified.

The sequence column order, the size of the columns and the hidden column configurations are saved with the sequence.

Some columns of the sequence have to be filled completely before the sequence is started: the method, Run name, Run ID, Run length, any mandatory user input variables if existing, the internal standards values and sample mass (if working in the corresponding calibration mode).

Once the sequence is filled, save it.

Multi Injector System

CompassCDS can acquire data on multi injector system. The sequence functioning is described below for a double injector.

If a system is composed of two injectors, the sequence works differently. In fact, two acquisitions are run simultaneously on one system. The sequence takes into account the two injectors.

Creation: During sequence creation, the user is asked to enter the number of lines. In the case of double injector, each injector will have the specified number of lines. The total number of lines of the sequence will be two times the specified one. For example, if a sequence is created with 7 lines, the first injector will be assigned 7 lines, the second injector 7 lines, and the whole sequence will have 14 lines.

Method column is not filled in as a single injector sequence. Both lines of the same run must be assigned with the same method. If the method field is entered for the first injector, the second injector one will be automatically copied.

Injector2 | Injector1 | ALL

Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections
1	☑	test.METH	inj2-	1	30	1
2	☑	test.METH	inj2-	2	30	1
3	☑	test.METH	inj2-	3	30	1
4	☑	test.METH	inj2-	4	30	1
5	☑	test.METH	inj2-	5	30	1

Sequence visualization: Three buttons change sequence displaying.

Injector1 Display only the first injector lines.

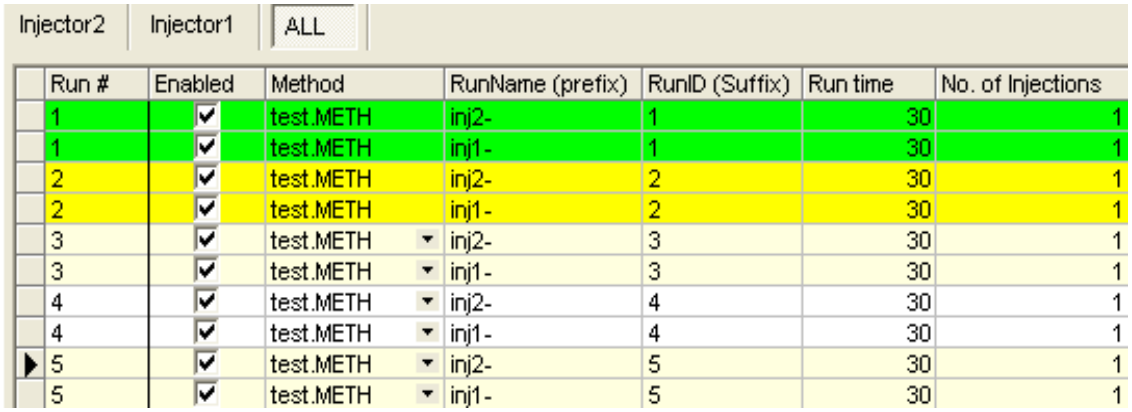
Injector2 Display only the second injector lines.

ALL Display all the lines of the sequence.

Number of lines: Respectively, the + and + buttons add or delete one run (Two lines). Each line corresponds to an injector.

Lines selection: If the two injectors have been selected in the method, every 'Enabled' boxes are active; they can be checked or unchecked according to user need. But if an injector has been unchecked in the method, the corresponding lines will be disabled and inactive in the sequence.

Acquisition: The Start ▶ Pause ❚❚ and Stop ■ buttons work simultaneously for both injectors. The two lines of the same run are acquired at the same time and are displayed in yellow when sequence is running.



If working in Specific Channel Parameters mode, (see acquisition part of the Method section), some variables (Multiplier and Divisor factors, sample mass, Istd values, and User inputs variables) are channel dependent. Meaning that for those variables a value must be entered for each channel (of each injector in the case of a multi injector system).

Some rules have to be taken into account to fill the sequence:

- Fill block for M, D Sample mass: It is best to fill the block from each injector screen, if entered from the ‘All’ screen the value of the first line will be copied on all channels of all injectors.
- Fill block for Istd and User inputs is realized by injector, the values entered for the first injector cannot be copied for the second injector.

Bracketing

With the normal calibration building mode, the standard chromatograms have to be acquired before the unknown ones. However, an option allows you to bracket the unknown chromatograms with standard runs:

To activate the bracketing option, open the sequence and check the ‘Bracketing’ box, in the top right part of the sequence. The Calibration column disappears and a Bracketing column appears.

To bracket samples by certain standards, fill the sequence in the acquisition order and enter the same bracketing identification, B1 for example, the following acquisitions can then be part of another bracketing.

Two bracketing can be overlaid:

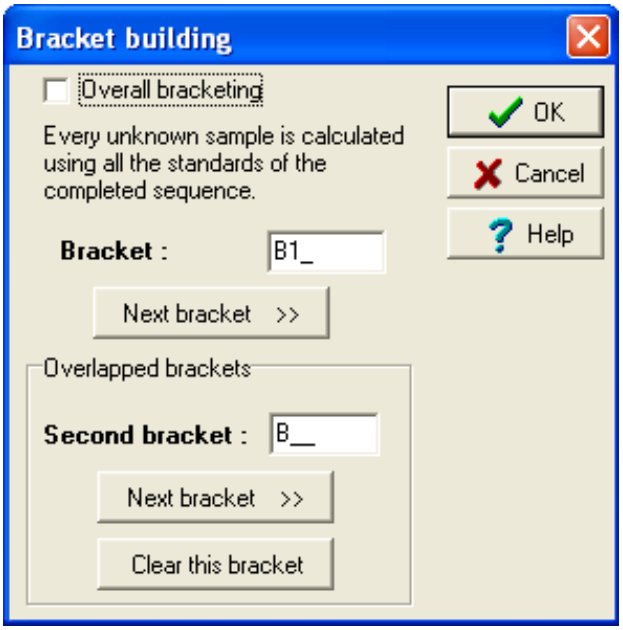
Run Suffix	Run ID	Standard	Level	Bracketing
Run	1	Standard	1	B1
Run	2	Standard	2	B1
Run	3	Unknown		B1
Run	4	Unknown		B1
Run	5	Standard	1	B1+B2
Run	6	Standard	2	B1+B2
Run	7	Unknown		B2
Run	8	Unknown		B2
Run	9	Standard	1	B2
Run	10	Standard	2	B2

The processing of the chromatograms acquired in sequence with bracketing is made after the acquisition of the whole sequence.

In the previous example the 10 injections are performed, then the calibration curve of the first bracketing is created with the four standard chromatograms Run1, Run2, Run5 and Run6. Then the first two unknown chromatograms (Run3 and Run4) are processed with this calibration curve.

This calibration curve is then archived and deleted and a second calibration curve is created with the four standard chromatograms Run5, Run6, Run9 and Run10. The last two unknown chromatograms (Run7 and Run8) are processed with this calibration curve.

To fill the bracketing column, enter the bracketing numbers separated with a ‘+’; for example ‘B1’, ‘B2’ or ‘B1+B2’ or use the button to access the following window:



This window allows you to easily fill in the bracketing column:

Check the 'Overall' bracketing box if the sample chromatograms should be created with a calibration curve containing all standards of the sequence.

Otherwise, for the first bracket enter B1_ and press the OK button. The cell is actualized with 'B1'.

Then for the second bracket, press the 'Next bracket >>' button. B1_ is changed in B2_ and press the OK button. The cell is actualized with 'B2'.

If the two brackets should overlay, press the 'Next bracket >>' button in the second bracket zone and press the OK button. The cell is actualized with 'B1+B2'.

NOTE: A maximum of 10 brackets can be defined. The use of bracketing is forbidden when using a multi-injector system or when selecting 'control sample' as sample type.

Use of System with a Prep-Ahead Sampler

If the system associated to the sequence is fitted out with a sampler which can prepare the sample to inject (mixing of sample, heating, stirring), a field allowing you to specify the maximum number of samples to prepare in advance is displayed above the grid of the sequence

.

Some restrictions are imposed in the sequence building and use:

- The same method must be defined for all lines
- The vials must be consecutive
- The same rack number must be defined for all lines
- Do not change the line order, add, delete insert or duplicate line, define multi injection per line or pause the sequence while it is running

NOTE: The preparation time of the sample is indicated in the Run Log of the chromatogram.

Running a Sequence

By pressing the Start icon, the sequence begins with the first acquisition.

It is possible to deactivate some of the acquisitions of the sequence by unchecking the 'Enable' cell of the corresponding lines.

If chromatograms already exist with the same file names, a warning message appears to inform the user that the files will be overwritten, or, if he does not own the corresponding right (profile defined in the Configuration Manager), forces him to change the chromatogram names.

When a sequence is started, the chromatograms are acquired one after the other in the defined order. The lines corresponding to chromatograms that are already acquired (or whose associated Enabled option is unchecked) are colored in green and the chromatogram that is being acquired is colored in yellow:

Injector2 | Injector1 | ALL

Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections
1	☑	test.METH	inj2-	1	30	1
1	☑	test.METH	inj1-	1	30	1
2	☑	test.METH	inj2-	2	30	1
2	☑	test.METH	inj1-	2	30	1
3	☑	test.METH	inj2-	3	30	1
3	☑	test.METH	inj1-	3	30	1
4	☑	test.METH	inj2-	4	30	1
4	☑	test.METH	inj1-	4	30	1
5	☑	test.METH	inj2-	5	30	1
5	☑	test.METH	inj1-	5	30	1

It is possible to insert additional acquisition lines (or modify existing lines) after the current chromatogram line that is being acquired (in yellow) during the sequence. Select the position of the new line to be inserted, and then click on the corresponding gray margin and select insert. A new line is inserted. To add a line at the end of the sequence, press . Fill it and the sequence lines will be acquired using the updated order. To remove a line, select it and press .

To insert an acquisition line just below the current line, it is better to first pause the sequence (icon). The current running sequence line continues until the specified acquisition time, but the next acquisition will not be started. To re-start the sequence, press the Start icon.

The Stop icon stops the sequence immediately.

To restart the sequence from the beginning, first press the Reset icon and then the Start icon .

NOTE: The sequence can be stopped automatically after a chromatogram process in case of Suitability test failure (see page 102), or Summary report variable test failure (warning or control) (see page 195). In both cases the user must have defined the 'Stop sequence' or 'Stop running sequence' action respectively for Suitability test and Summary report.

NOTE: If the user profile contains the right ‘Enable automatic save’, in the sequence section, a sequence file is automatically created each time a sequence was performed. This new sequence (which is a copy of the original one) is named sequencename_timestamp.SEQU (where sequencename is the name of the original sequence). This option has to be selected if the user wants to:

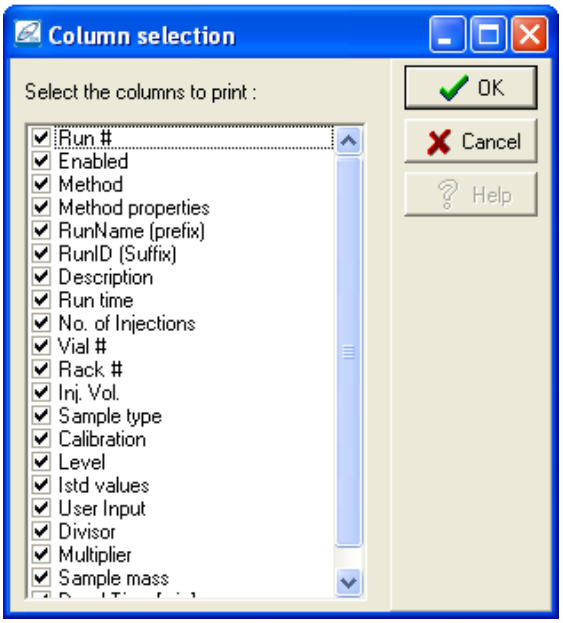
- sign a batch of chromatograms coming ‘from a sequence’

- create a REPL from a sequence, in the case a token was defined in the chromatogram name generation (acquisition parameter) (for example’ $Projectname-$AcqMethodName’, especially if the sequence was run as a remote sequence.

Printing a Sequence

When a sequence is opened and selected, press the icon or select the menu FILE / PRINT.

The following window appears:



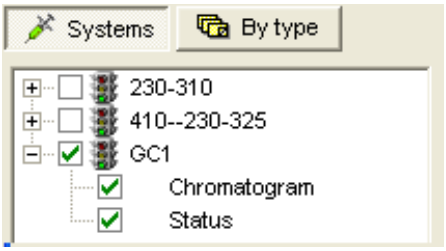
This window lists all the sequence columns. Check only the columns to be printed and press the OK button.

The sequence is printed.

Viewing an Acquisition

To view a chromatogram during its acquisition, select the ‘Systems’ tab. In the main screen, all the systems defined in the project in which user is connected are listed in the browser. If connected in “all projects”, all the systems defined in the group are listed.

In the browser, select the system(s) to view, the name is then preceded by and the selected system(s) is (are) automatically displayed. A tab is created for each new system in the right part of the screen. In the case of multi injector, visualization remains identical.



An idle system is preceded by the symbol, a system which is downloading the method or is waiting for the injection by , and a running system by .

To remove a view, uncheck the system performing the acquisition in the browser, the tab associated to the system is automatically removed.

Selecting the Information to Display

Select the “Systems” tab in the browser.

The acquisitions can be displayed system by system, or the same information can be displayed for several acquisitions on the same page.

Click on Systems to display all the information concerning an acquisition on a single page. Click on By type to display the information concerning the acquisitions according to type. (For example, all the chromatograms or the system status information, or both).

- System mode

In the browser, all systems that the user is allowed to control are listed (the list depends on the project of the user).

For each system, there are two sections: Chromatogram and Status.

If Chromatogram is checked for a particular system, a page is created containing the chromatogram. If Chromatogram and status for another system are checked, the new page will be separated between the section for the chromatogram and the section for the status.

- By type mode

There are two sections in the browser: Chromatogram and Status.

In each section (chromatogram and status), all systems which the user is allowed to control are listed.

If all the systems are checked, they will be displayed together. Four chromatograms can be displayed on each page, so if there are more than four selected systems, the other chromatograms will be displayed on a new page.

NOTE: It is best to not simultaneously view a large number of chromatograms or status. Doing so could lead to a problem with a virtual memory leak.

When “Status” is checked, information regarding the status of the acquisition system is displayed. The display will differ, depending upon the exact system configuration, e.g., whether the chromatograph is using full control drivers, etc.

If the system is not unchecked, and a new acquisition is started, the new acquisition will be displayed in the same window.

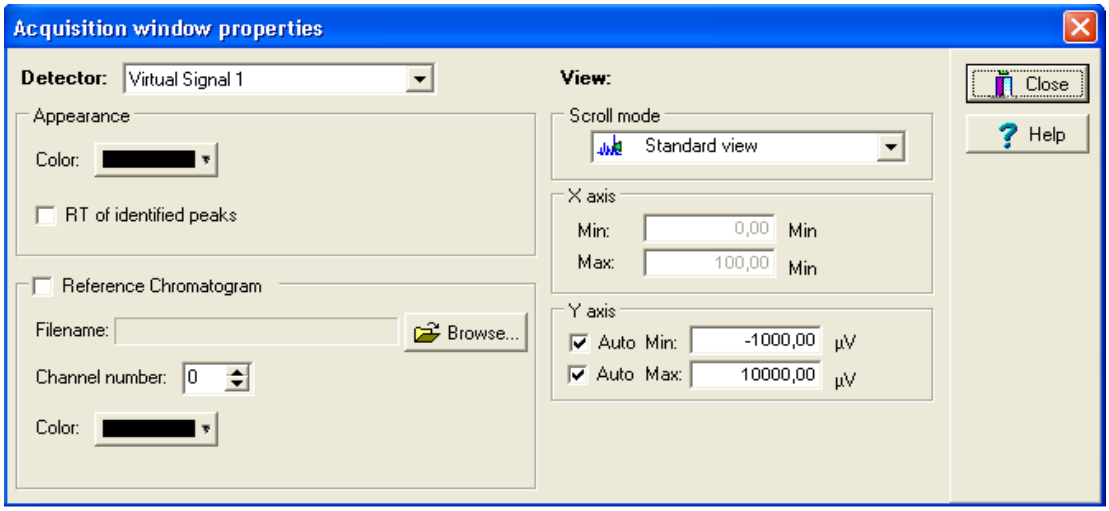
The Acquisition Window

The Tasks Bar

	Stops the current run. If the instrument is fully controlled, CompassCDS does not receive any information that the instrument is stopped. It is therefore necessary to stop the run within the software. CompassCDS will ask for a confirmation before stopping a run. Only the person who started an acquisition has the right to stop it, except some users that have the right to stop any running acquisition. This level of privilege is defined in CompassCDS Configuration Manager.
	Modifies the acquisition time. Note that by decreasing the acquisition time to a value less than the current run time, the acquisition will be stopped.
	Displays the chromatogram with automatic scaling: both scales are continuously updated after each acquisition points, such that the entire chromatogram is displayed.
	Displays the chromatogram in a fixed window. The parameters can be changed in the properties (see the corresponding icon below).
	Sets the parameters for the x-scale that moves along as the acquisition runs. It is possible to view only the last minute of acquisition, for example. To modify the width of this window, use the properties (see the corresponding icon below) and in the scrolling section, it is possible to change this default value.
	This icon is useful if there are several traces (several detectors) to stack the view of the two acquired chromatograms.
	This icon is useful if there are several traces (several detectors) to overlay the two acquired chromatograms.
	This icon synchronizes X axis of acquiring chromatograms. If one chromatogram is zoomed or moved, every chromatograms of the acquisition window will be also zoomed and moved.
	This icon modifies the acquisition view properties.

Acquisition View Properties

To look at the chromatogram viewing properties during acquisition, click on the icon. First, select the chromatogram to modify. The following window appears:

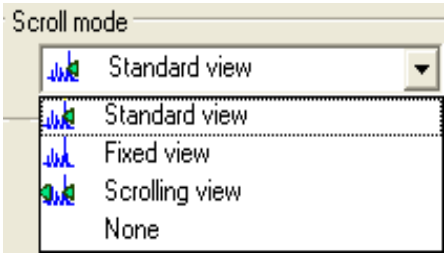


It is possible to define the colors of the chromatogram trace. To modify the colors of a trace, select the chromatogram channel to be modified in the 'Detector' zone, and then click on the color box to select the new color.

If peaks have been identified in the acquisition method (peaks identification section), it is possible to display their theoretical identification window on the chromatogram during acquisition. Select ‘RT of identified peaks’ option.

It is also possible to display a chromatogram as a reference. The new chromatogram will be overlaid with the reference. Press the Open icon ( ) and select the chromatogram to overlay in the Open file window and the chromatogram channel to overlay with the 1 box. To hide the reference chromatogram for a moment, uncheck the Reference chromatogram option.

- In the ‘Scroll mode’ zone, select the acquisition view:



Standard view: In this view, the X-scale is updated to the current acquisition time so that only the already acquired section is viewed. The Y- scale is automatic by default, but fixed limits can also be set (in the Y axis zone by un-checking the Auto option). An automatic scale means that the minimum is set to the minimum signal value and the maximum is set to the maximum signal value: the Y-scale is large enough to display all the acquisition points.

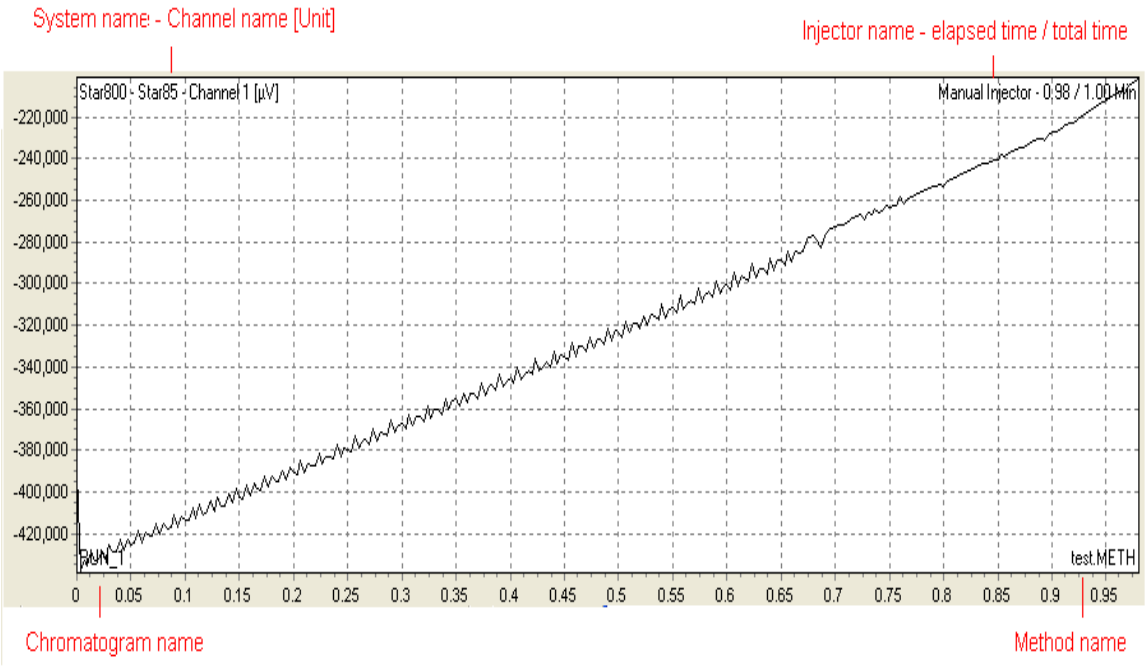
Fixed view: In this view, the X-scale is fixed, by default between zero and the expected acquisition time. The Y-scale is automatic by default, but if ‘Auto’ is unchecked, the corresponding values are set as fixed limits. The limits of the X-scale can be changed in the X axis field.

Scrolling view: This view shows only the last acquired points, within a width defined in the ‘Scrolling’ field. By default, the last acquired minute is shown. The Y-scale is either fixed or automatic.

Acquisition view display

Chromatogram plot and the following information are displayed on the acquisition view:

- System name - Channel name [Unit]
- Injector name – Elapsed time /total time
- Chromatogram name
- Method name



Acquisition Directory

It is possible to save the chromatograms in a different directory each day or in a directory depending on the instrument or user that performed the acquisition, etc. The special directories, which can be created to save the chromatograms, are called token.

For example you can start the same sequence with the same chromatograms every day but, save them in a directory named after the actual date.

Token mode is defined, thanks to a profile defined in the CompassCDS Configuration Manager.

Stop or Start a System

It is possible to stop or start a system from CompassCDS, as it is in CompassCDS Configuration Manager. The functions are available via the Systems tab: select a system and click on start or stop in the popup menu (double-click on the right mouse button). This option has to be set in the profile in CompassCDS Configuration Manager (Acquisitions / System properties / Allow to start or stop systems).

When stopping a system, the corresponding service is stopped, the system is idle. The start function starts the service associated to the system. It can be useful to stop a system without opening CompassCDS Configuration Manager, to carry out maintenance operations.

Exiting the CompassCDS Chromatography Data System

(While an Acquisition is running)

If a sequence is running, it is not possible to close CompassCDS. If Quick Start is actively running and CompassCDS is closed, the acquisition will continue and be saved, but will not be processed (note that the report will not be printed). The chromatogram will then be processed as soon as it will be opened within CompassCDS.

The Calibration Curves

A calibration curve consists of a series of individual calibration curves for each compound. The file is identified by a specific name.

For example, assume that there are three compounds in standard chromatograms, e.g. Glycine, Arginine, and Methionine, and the corresponding calibration curve is named ‘Amino Acids’. There will be a global calibration curve called ‘Amino Acids’, which will contain three calibration curves: one for ‘Glycine’, one for ‘Arginine’ and the last curve for ‘Methionine’.

Calibration curve Configuration

The calibration curve configuration is defined in CompassCDS Configuration Manager: the calibration curve can plot either quantities versus responses (area, height, area%, height%, $area^{1/2}$, and $height^{1/2}$) or responses versus quantities.

Building a Calibration Automatically

To create a calibration curve, the calibration method must be configured correctly (see page 76). Define at least the following parameters.

1. Select ‘Curve’ in the Factor list box.

   Specify the name of the calibration curve in the Calibration curve / File field and the unit of the standards in the Standard / Unit field.
   Complete the calibration table:

   Define the regression models and point-weighting mode.

   Define the number of compounds for each level in the standard sample table.

   When the method has been created and saved, it can be used to create calibration points.

2. If the standard chromatograms have already been acquired:

   Open the chromatograms to reprocess and then select the PROCESSING / REPROCESS menu. In the Reprocessing window, select the name of the first standard chromatogram and the name of the method.

   Now, select the appropriate calibration level from the calibration table column. This level should display the same standard amounts which correspond to the current sample standard amounts. Check ‘Clear old points’ to delete all the existing calibration points or check ‘Clear this level only’ to delete only those calibration points corresponding to the same calibration level. To add the calibration point to an existing curve, do not check anything. The cleared calibration points are not completely deleted, but archived.

   Now press ‘Reprocess’ to add the points.

Repeat the operations for all standard chromatograms (or use a reprocessing list, see page 173), take care to uncheck the boxes 'clear old points' or 'clear this level only' to add the next points, then close.

When the calibration curve has been created, open the Calibration page to view the results.

If the standard chromatograms have not been acquired:

Select the ACQUISITION / QUICK START menu options. Select the appropriate chromatograph and method, and then fill in the acquisition parameters in the Quick Start window.

In the Calibration section, select the appropriate calibration level, according to the values entered in the calibration table. Check ‘Clear old points’ to delete all the existing calibration points or check ‘Clear this level only’ to delete only those calibration points corresponding to the same calibration level. To add the calibration point to an existing curve, do not check anything. The cleared calibration points are not completely deleted, but archived.

The acquisition can now be started.

Repeat the operations for all the standard chromatograms and then close.

A calibration curve can also be created automatically during a sequence.

Building a Calibration Curve Manually

It is possible to add calibration points without using a standard chromatogram by entering point coordinates or by using a curve equation.

Open calibration curves, in the calibration point table, right click and select ADD POINT MANUALLY or ADD POINT FROM EQUATION. A window will appear which contains two tabs: ‘From equation’ and ‘manually’.

- Manual point addition.

  In the “Manually” page, select the number of points to be added.

  For each point, enter the response in the corresponding column and the amount in the other column.

  Select the calibration level corresponding to the points. The level will be useful if adding calibration points from a calibration chromatogram after the manual entries. If the level of the manually added point is X and ‘average level’ is checked in the method calibration part, this point is taken into account in the average calculation. When a level X point is added, if ‘Delete this level only’ is checked, the manually added point will be canceled.

  Press the OK button.

- Point addition from an equation:
- In the ‘From equation’ page, enter the curve equation from the drop-down list. Some existing linear equations are already entered for convenience. All that is needed is the replacement of the polynomial coefficients in the existing equations. The sign ‘^’ means ‘to the power of’

  Select the number of points to be added.

  For each point, enter the response or the quantity (according to the calibration curve orientation) in the corresponding column and then press Compute. The amount

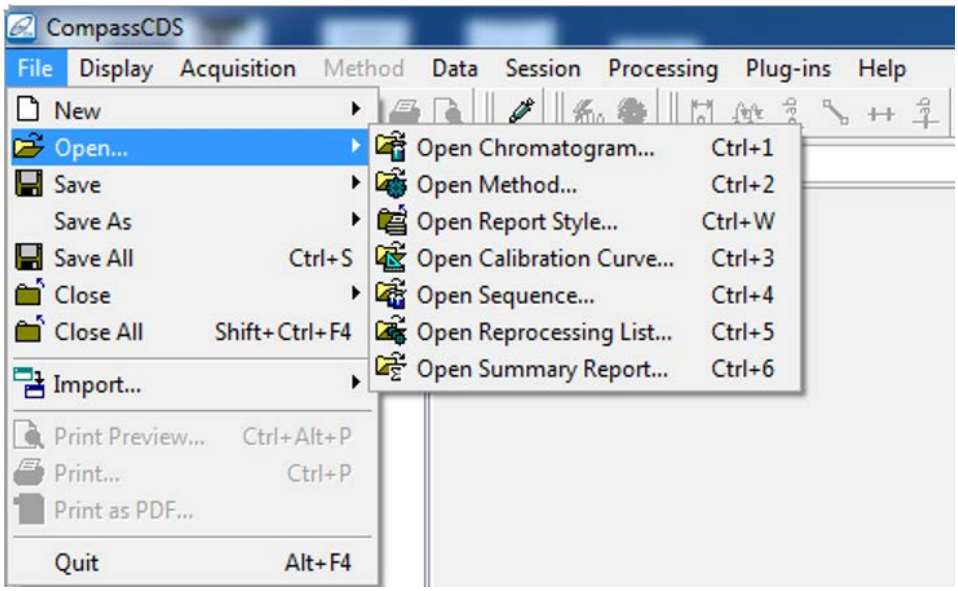
corresponding to the response in the equation is calculated, and displayed in the other column.

Select the calibration level corresponding to the points. The level will be useful if adding calibration points from a calibration chromatogram after the manual entries.

Press the OK button.

Displaying a Calibration Curve

To view a calibration curve, select the FILE / OPEN / OPEN CALIBRATION CURVE menu or use the icon “Open” and choose OPEN CALIBRATION CURVE in the sub menu.

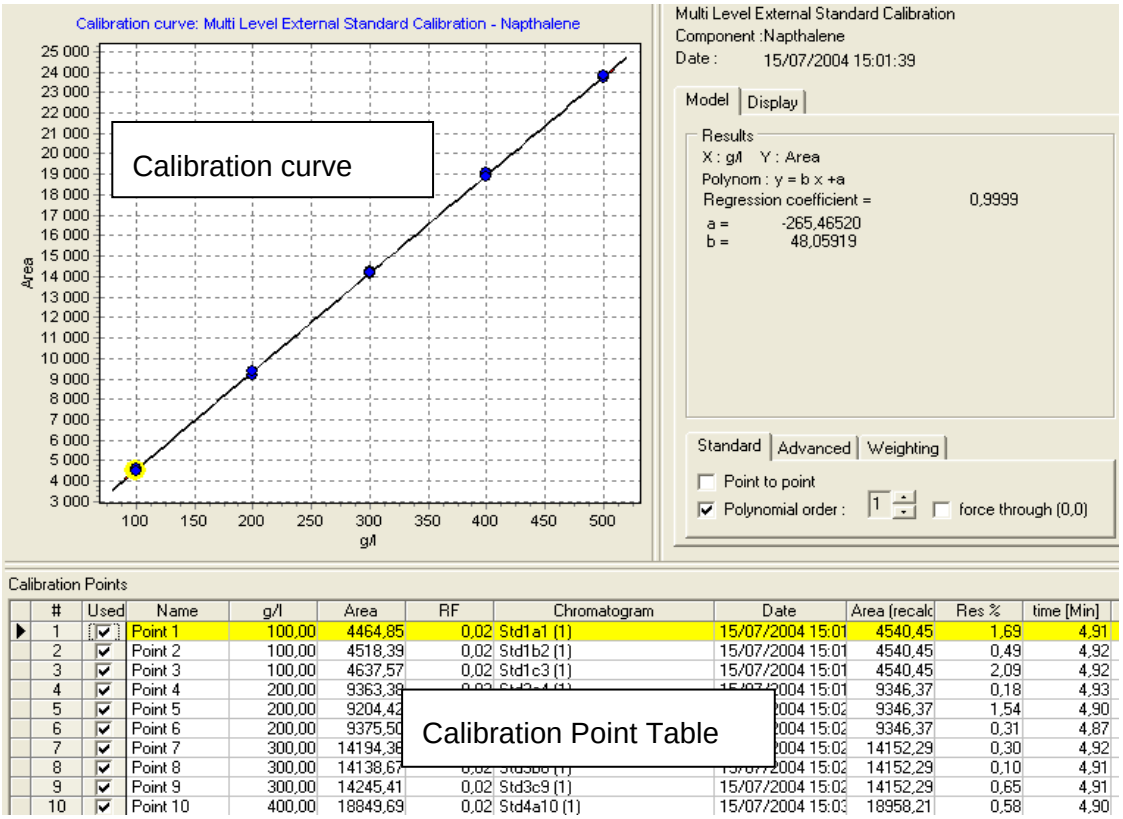


The calibration curves of all the compounds are listed in the browser.

When selecting a compound in the browser, the calibration curve of the corresponding component is displayed in the right panel.

Close to the plot are shown

- The global name of the curve, which is the file containing the calibration curves of every compound in the standard chromatogram.
- The name of the compound itself.
- The last date and time of modification.



#	Used	Name	g/l	Area	RF	Chromatogram	Date	Area (recalc	Res %	time [Min]
1	☑	Point 1	100,00	4464,85	0,02	Std1a1 (1)	15/07/2004 15:01	4540,45	1,69	4,91
2	☑	Point 2	100,00	4518,39	0,02	Std1b2 (1)	15/07/2004 15:01	4540,45	0,49	4,92
3	☑	Point 3	100,00	4637,57	0,02	Std1c3 (1)	15/07/2004 15:01	4540,45	2,09	4,92
4	☑	Point 4	200,00	9363,39			15/07/2004 15:01	9346,37	0,18	4,93
5	☑	Point 5	200,00	9204,42			2004 15:02	9346,37	1,54	4,90
6	☑	Point 6	200,00	9375,50			2004 15:02	9346,37	0,31	4,87
7	☑	Point 7	300,00	14194,36			2004 15:02	14152,29	0,30	4,92
8	☑	Point 8	300,00	14138,67			2004 15:02	14152,29	0,10	4,91
9	☑	Point 9	300,00	14245,41	0,02	Std3c9 (1)	15/07/2004 15:02	14152,29	0,65	4,91
10	☑	Point 10	400,00	18849,69	0,02	Std4a10 (1)	15/07/2004 15:03	18958,21	0,58	4,90

- The calibration curve

In this curve, the calibration points are shown and the regression model is drawn.

In this curve, as in chromatograms, both zoom in and zoom out functions are available. The curve may be copied to the Clipboard, and the graphic properties can be changed.

- It is possible to zoom in on the graphs by pressing the left mouse button in the top left-hand corner of the area to magnify and keeping it pressed until the bottom right-hand corner is reached.
- If the left mouse button is clicked, then dragged from the bottom right-hand to the top left-hand corners, the graph is brought back to full scale.
- A right mouse click within the graph area will display a popup menu with the following options:

Full scale: Returns graph to full scale.

Zoom in: Returns graph to the previous zoom in.

Zoom out: Returns graph to the previous zoom out.

Copy: Copies the curve as it appears on the screen (in order to paste it into another application using the local paste function).

Properties: Accesses the curve properties to modify its display.

NOTE: When the Average RF model is chosen, the curve shows the response factor (RF) versus the different calibration points (# point).

- The Model panel

The regression model is displayed in the Model panel with parameters quantifying the integrity of the regression. The regression model can be modified and the curve will be automatically recalculated.

- In the Model panel, the following elements are displayed:

The results, which are the theoretical equation of the regression curve, include the regression coefficient, and the numerical value of the equation coefficients (a, b, c, etc.)

NOTE-1: The method of least squares (or ordinary least squares) is used to calculate this regression coefficient.

The calculation is slightly different from the one in Excel®:

Excel®: $1-\frac{\sum(y-\hat{y})^2}{\sum(\bar{y}-y)^2}$

CompassCDS: $\frac{\sum(\hat{y}-\bar{y})^2}{\sum(\hat{y}-\bar{y})^2+\sum(y-\hat{y})^2}$

Where:

$\hat{y}$: is the standard deviation

$\bar{y}$: is the average

NOTE 2: If the Average RF model is chosen, the following curve related variables are displayed:

RF= Average response factor:

$$RF = \sum_{i=1}^{N} \frac{Q_i}{R_i}$$

RSD= Response factor_Standard deviation

$$RSD = \sqrt{\sum_{i=1}^{N} \frac{1}{N-1}\left(RF_i - RF\right)^2}$$

%RSD= Response factor_Relative Standard deviation

$$\%RSD = \frac{RSD \times 100}{RF}$$

N= the number of calibration points

It is possible to modify the regression model in this panel and to immediately view the results of the entire page (calculation of the regression curve and coefficient, curve display).

Different regression models are available:

Standard:

Point to point: The calibration curve is composed of lines drawn between the calibration points.

Polynomial: It is possible to modify the order of the polynomial. A calibration curve can be modeled with up to a 5th order polynomial. The polynomial regression can be forced through zero (for example, in case of a one-point calibration, the polynomial will be of order one and forced though zero).

If there are not enough points for the calculation (e.g. only one point available for a 2nd order polynomial), the order of the polynomial is reduced, and a message is displayed in the panel (below the polynomial coefficients).

It is possible to force the curve to go through (0, 0) by checking the corresponding option.

Advanced:

Power: this is a $\mathbf{y=ax^b}$ model.

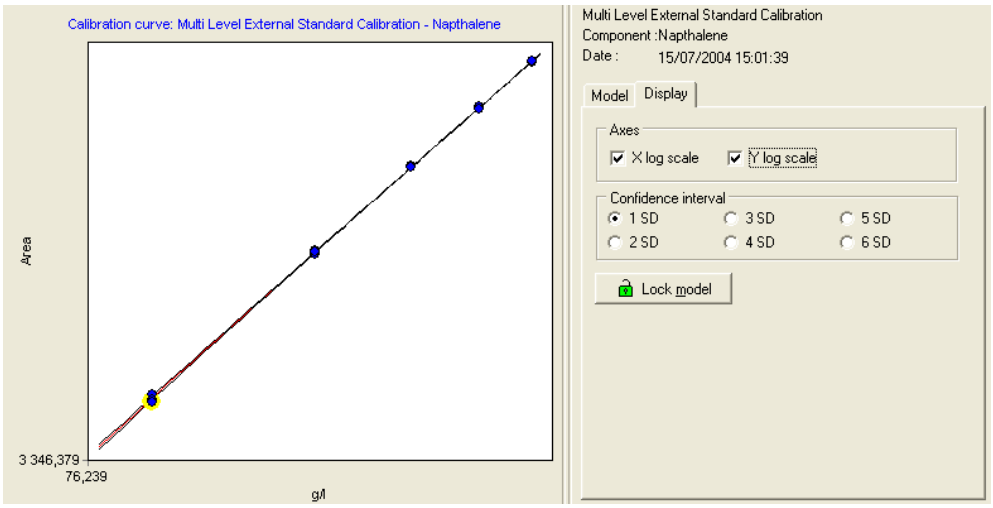
Exponential: this is a $y=a\ e^{bx}$ model.

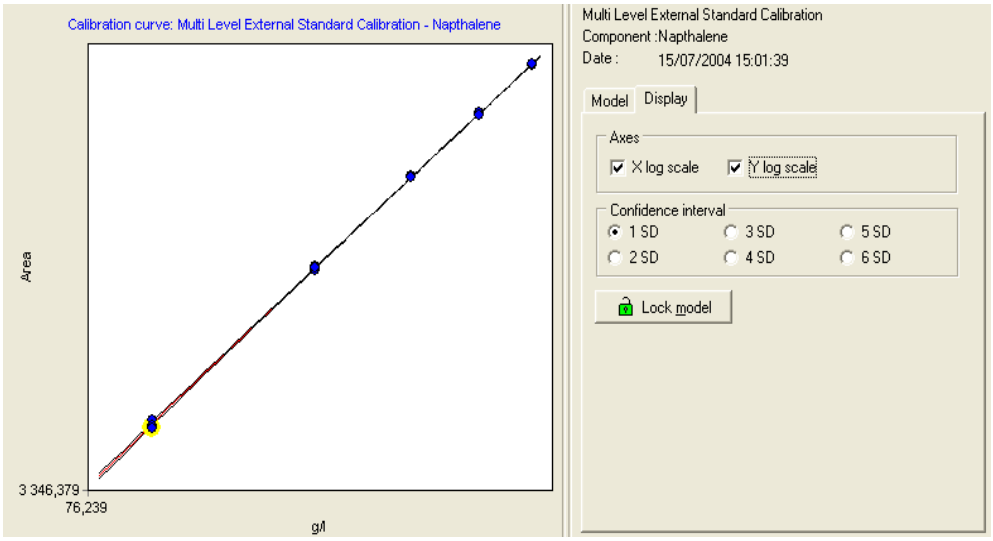
Logarithm: this is a y=a + b ln x model.

Average RF: If that model is chosen, it will imply automatically a linear model, force (0, 0) and $1/x^2$ weighting for the curve building. When the Averaged RF model is chosen, the other options which are set automatically cannot be changed until the calibration mode is changed.

- The Display panel

For both Standard and Advanced modes, it is possible to display the logarithm axis scales, by checking the X log scale or/and Y log scale boxes. These options can be interesting for curves for which the regression model is a power for example, it enables to view curve under a linear model, as displayed in the following example:





The confidence intervals can be chosen by the user (between 1 and 6 SD-Standard Deviation). Those intervals are displayed whatever the chosen model (linear, polynomial, etc.)

A Lock Model button can be found at the bottom of the panel. This locks the calibration curve after it has been validated.

Different weighting models are available:

None: This assigns the same importance to all calibration points.

x: This model calculates each calibration point using a weight proportional to the abscissa of the curve.

x^2: This model calculates each calibration point using a weight proportional to the square of the abscissa.

1/x: This model calculates each calibration point using a weight proportional to the inverse of the abscissa.

$1/x^2$: This model calculates each calibration point using a weight proportional to the square of the abscissa inverse.

log x: This model calculates each calibration point using a weight proportional to the decimal logarithm of the abscissa

ln x: This model calculates each calibration point using a weight proportional to the natural logarithm of the abscissa.

1-N: The weight of each new point is equal to the sum of previous point weights. For example, for 5 points, the weights are respectively: 1, 1, 2, 4, 8.

- The calibration points table

This is a table containing all calibration points with information about the source chromatogram and their addition.

#: Index

Used: Check or uncheck the boxes to activate or deactivate the calibration points.

Name: The name of the point corresponding to the order of addition.

Response: This column is the response (area or height) of the peak or the response of the compound divided by the response of the corresponding internal standard.

Quantity: This column is the compound amount or the compound amount divided by the corresponding internal standard amount.

RF: This column gives the response factor of the peak.

Chromatogram: This is the name of the source chromatogram from which the calibration point was added followed by its acquisition channel number in parenthesis. If the point was created manually, the cell content is “User defined”. If the point was added from a curve, the cell content is based on the curve equation.

Date: This column gives the point addition date and time.

Recalculated quantity: This column displays the projection of the calibration point where the quantity is recalculated to fall on the regression curve while maintaining the same response.

Res%: The residual standard percentage. It is calculated with the following formula:

$$\mathrm{Res\%} = \frac{y - \bar{y}}{y} \times 100$$

Where

y Is the quantity entered in the calibration table

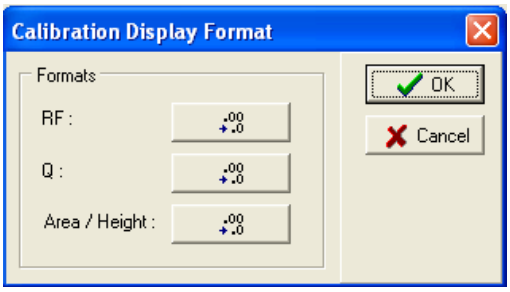
$\bar{y}$ Is the recalculated quantity

Time: The retention time of the peak corresponding to the compound in the standard chromatogram.

Level: The level defined in the calibration method. This is the level specified before the acquisition or the reprocessing

Username: The name of the user who created the calibration point.

NOTE: The format of the response factors, the response and the retention time can be modified. Right click in the calibration result table and choose the Format menu. The following screen appears:



Click on the variable you want to modify the format:

The new format is applied only in the calibration result table and in the Model panel for the RF.

- Activating and deactivating the points

Some calibration points can be far from the calibration curve (check the residual percentage). In this case, deactivate them, and the regression model is automatically recalculated without these points. Save the curve to use it for unknown samples.

There are two ways to deactivate or reactivate a point:

- In the calibration point table at the bottom of the panel, check or uncheck the “Used” boxes to activate or deactivate the calibration points. The last possibility is to double-click on the point in the browser.

A deactivated point is displayed in gray in the curve, the ‘Used’ box is unchecked in the calibration point table, and the icon is displayed in the browser.

An activated point is displayed in blue in the curve, the ‘Used’ box is checked in the calibration point table and the icon is displayed in the browser.

The Archives

Calibration curves are archived only if the corresponding profile has been associated with the user in the CompassCDS Configuration Manager (User profile, 21CFR11-user / Audit Trail / Archive Calibration Curve).

An archive is created, each time a point is added in the calibration curve.

The archives can be displayed either by component or by date.

Click on the

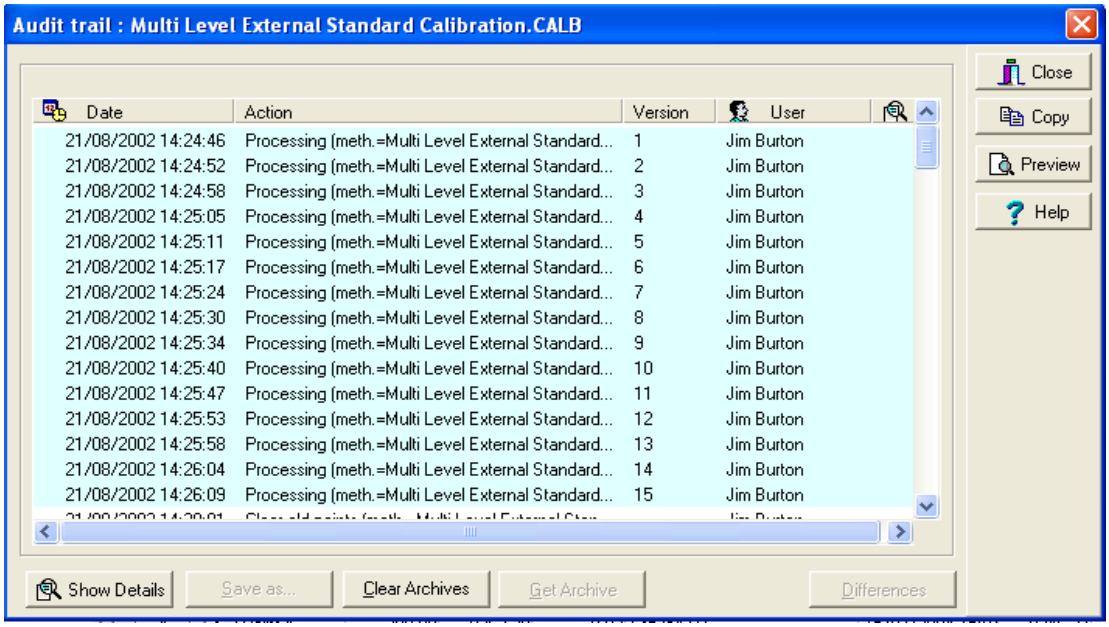
button to display them by component, or click on the

button to display them by date.

Click on the name or the date of the archives to display it in the right panel. The calibration curves are locked once they have been archived but the calibration point values and the regression model parameters can be viewed.

NOTE: The displayed archiving date does not correspond to the curve creation date but to the date on which it was replaced by another one, i.e., the curve creation date of the new calibration curve.

Note that an archived calibration curve can be used to reprocess chromatograms. Consult the Audit trail of the curve ( ):

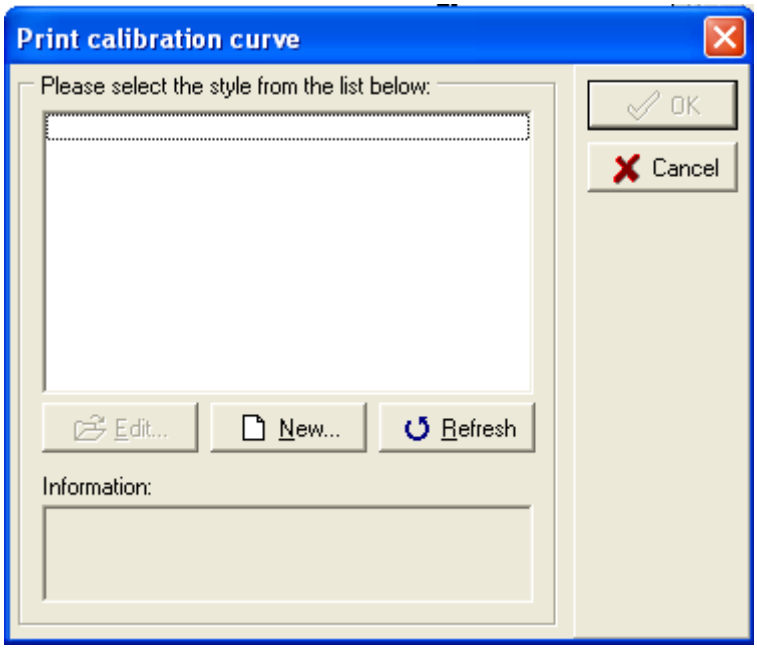

Audit trail : Multi Level External Standard Calibration.CALB
Close
Copy
Preview
Help
Date
Action
Version
User
21/08/2002 14:24:46 Processing (meth.=Multi Level External Standard... 1 Jim Burton
21/08/2002 14:24:52 Processing (meth.=Multi Level External Standard... 2 Jim Burton
21/08/2002 14:24:58 Processing (meth.=Multi Level External Standard... 3 Jim Burton
21/08/2002 14:25:05 Processing (meth.=Multi Level External Standard... 4 Jim Burton
21/08/2002 14:25:11 Processing (meth.=Multi Level External Standard... 5 Jim Burton
21/08/2002 14:25:17 Processing (meth.=Multi Level External Standard... 6 Jim Burton
21/08/2002 14:25:24 Processing (meth.=Multi Level External Standard... 7 Jim Burton
21/08/2002 14:25:30 Processing (meth.=Multi Level External Standard... 8 Jim Burton
21/08/2002 14:25:34 Processing (meth.=Multi Level External Standard... 9 Jim Burton
21/08/2002 14:25:40 Processing (meth.=Multi Level External Standard... 10 Jim Burton
21/08/2002 14:25:47 Processing (meth.=Multi Level External Standard... 11 Jim Burton
21/08/2002 14:25:53 Processing (meth.=Multi Level External Standard... 12 Jim Burton
21/08/2002 14:25:58 Processing (meth.=Multi Level External Standard... 13 Jim Burton
21/08/2002 14:26:04 Processing (meth.=Multi Level External Standard... 14 Jim Burton
21/08/2002 14:26:09 Processing (meth.=Multi Level External Standard... 15 Jim Burton
Show Details
Save as...
Clear Archives
Get Archive
Differences

Click on the Get archive button (if your profile allows you to do this operation). The current calibration curve is then replaced by the old one.

The user can also save a calibration curve archive under a new name thanks to the ‘Save as…’ option.

Printing a Calibration Curve

To print a calibration curve, open it then click on the icon. The following screen is displayed:



The user selects a defined report in the list, he can edit it by pressing the Edit button, create a new one by pressing the New button to customize the report, or refresh the list by pressing the Refresh button.

Manual Integration and Identification

Manual Identification

If the peaks are not well identified, it is possible to rename them manually within the peak report table (peak results).

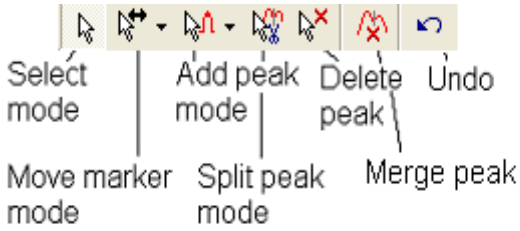
Double-click on the Name cell for the line of the peak to be renamed. Type the name of the peak in this cell.

If some reference peaks are identified manually the non-reference peaks will be identified according to the new reference times.

Manual Integration

The manual integration toolbar helps you to define the peaks manually (modify their start and stop time, delete or add…), the same modifications can be made within the peak results table, by changing manually the start and end retention times of peaks.

If the manual integration toolbar is hidden, select the DISPLAY / TOOLBARS menu and check Integration. The toolbar appears:



- Select mode

  This is the normal mode. If Select mode is pressed, it is possible to click on the markers in the graph to select them.

  Another possibility is to click on the corresponding peak in the peak result table.

  The third possibility is to press the right mouse button within the peak (in the graph), then choose PEAK / SELECT in the popup menu.

  The selected peak is highlighted in yellow in the peak result table, and its markers are highlighted in yellow in the graph.

- Move marker mode

  Press this icon to move a marker manually in the graph. Click on the marker to be moved, and then click a second time on the marker's new location on the graph.

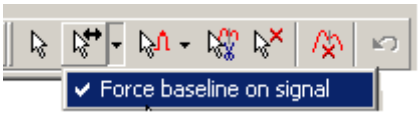
  Another possibility is to display the Start and End columns in the peak result table and to manually enter their new position.

  A marker cannot be moved before the previous marker or after the following marker.

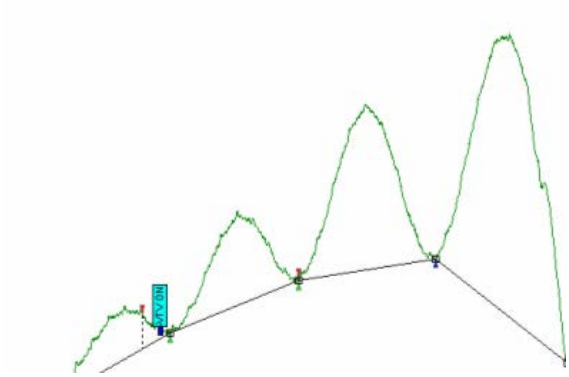
  Use the Move marker mode to move the integration events or the baseline. To move the baseline without the peak markers, hide the peak markers (press the display peak markers

icon) and move the markers symbolizing the edges of the baseline as for the other markers.

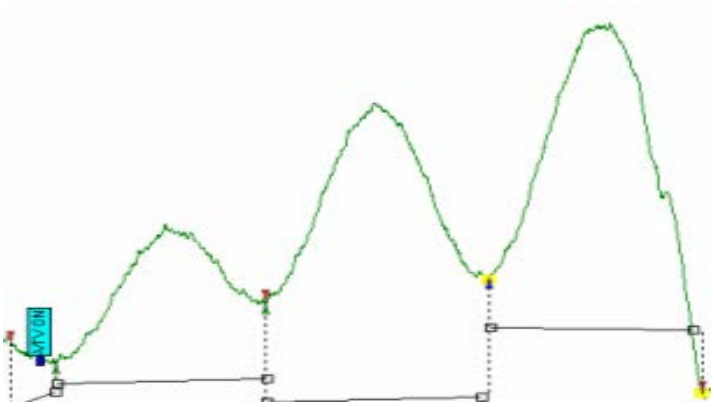
It is also possible to enforce or not the baseline on signal:



When the Force baseline on signal option is used, the baseline markers are always attached on the signal.



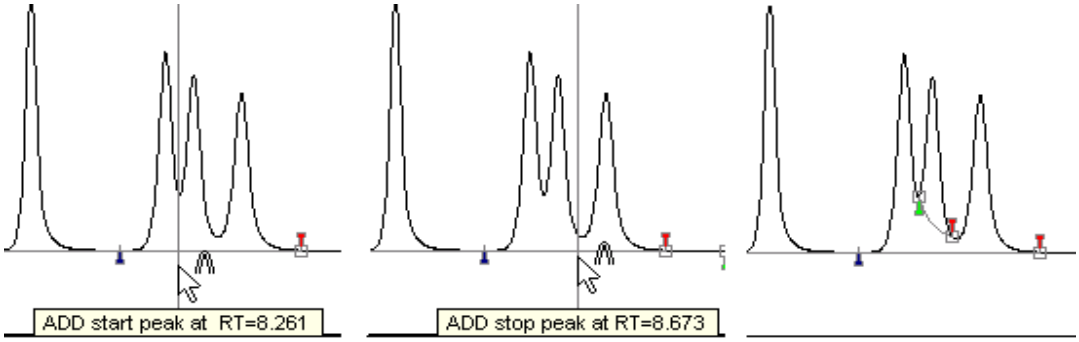
If that option is unchecked, it is possible to put the baseline marker wherever you want:



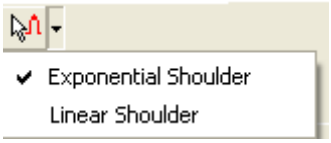
- Add peak mode

  Press this icon to add a peak. Click on the location of the start marker, and then click on the location of the end marker.

  If the two markers are added inside a peak, a shoulder peak is created:



The baseline of shoulder peaks is always a line, either exponential or linear. It is possible to define the shoulder integration mode (tangential or exponential) before moving markers, in the sub menu of the icon:



- Split peak mode

  Press this icon to split a peak. Click the left mouse button at the point where the peak should be split, and a valley marker is created at this location.

  Another possibility is to press the right mouse button at the point where the peak should be split, then select the PEAK / SPLIT option from the appearing popup menu.

  A shoulder peak (or a mother peak) can be manually split.

- Delete peak

  Select one peak (in the graph or in the table) as described above, then press the Delete peak icon.

  Another possibility is to first select the peak, then press the right mouse button within the peak result table, and select DELETE CURRENT PEAK from the popup menu.

  The peak that will be deleted using the two possibilities described above is the selected peak. This means that the peak highlighted in yellow within the peak result table and whose markers are highlighted in yellow within the graph is deleted.

  The third possibility is to press the right mouse button within the peak in the graph and then select PEAK /DELETE from the popup menu.

- Merge peaks mode

  Select one peak (in the graph or in the table) that as has been split into 2 peaks or that has a common marker with another peak (valley), then press the Merge peaks icon. The current peak is deleted and the next peak is extended to the left in order to include the deleted peak.

- Undo

  Press this icon to undo the previous manual action.

Manual Operation History

All the manual operations performed are listed in the chromatogram file.

Click on Results, then Manual operation in the browser to view the manual operation history displayed in the right panel.

The manual operations are either manual integration or manual identification.

The date and time of the operations are listed, along with the nature of the modification that was made.

Press the right mouse button in this panel and select UNDO LAST ACTION in the popup menu to cancel manual operations one after the other.

When saving a manually modified chromatogram, the manual operations are saved along with this history.

NOTE: It is possible to print the manual operation list in the report.

Modifications due to Manual Operations

When a peak is added or when the markers of a peak are moved, the variables are updated with the new response values.

But, if the chromatogram is a standard one, the modifications are not automatically taken into account. It will be necessary to create some calibration points with this chromatogram again, and to deactivate the previous ones. Enter the Reprocessing window to add the points (PROCESSING / REPROCESS) and open the calibration curve in the corresponding tab set (FILE / OPEN / OPEN CALIBRATION CURVE) to deactivate the points.

NOTE: To reprocess a chromatogram, without losing the manual integration, select the menu PROCESSING / REPROCESS, uncheck the Clear Manual Operation box in the options page and reprocess the chromatogram.

Reprocessing a Chromatogram

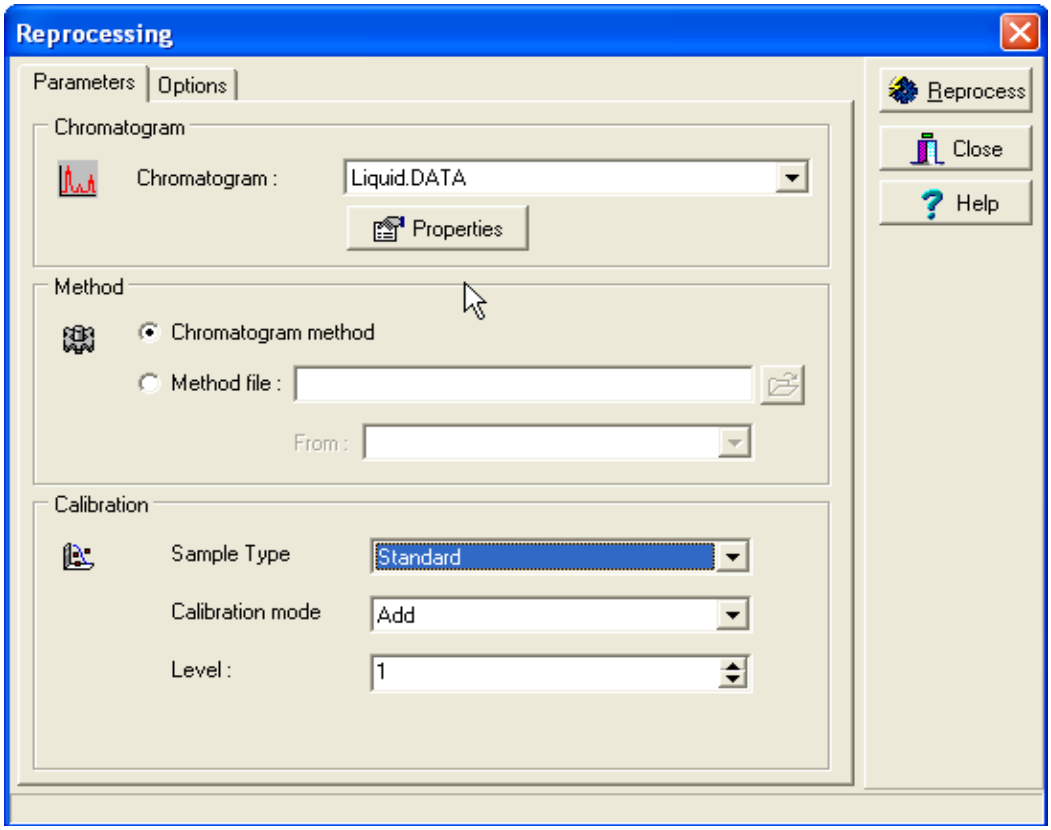
Once a chromatogram has been acquired, it is possible to reprocess it with another method. The previous method will not be lost but will be saved in the Audit Trail, if this function is defined in the CompassCDS Configuration Manager. For each processing or reprocessing a copy of the file is saved with the name of the user doing the processing. This file can be recovered (see Audit Trail page 204).

Single Reprocessing

The chromatogram should be opened in CompassCDS to be reprocessed in the single reprocessing window.

Choose the menu PROCESSING / REPROCESS to access the reprocessing window:

The 'Parameters' tab



In the Chromatogram zone, select the chromatogram file to reprocess from the list of all the chromatograms opened in CompassCDS.

If some properties of the chromatogram have to be changed before the reprocess (multiplier factor, divisor factor, sample mass, internal standard values, dead time) click on the Properties button and define the new values.

Then choose the method in the corresponding field. If 'Chromatogram method' is chosen, the method from the chromatogram file is used. If another method should be used, choose 'Method file' and press the open icon ( ) in order to choose a method.

In the Calibration section, define in the Sample Type field whether the chromatogram is a blank, an unknown, a standard, a control sample or a control sample of level-I. According to the option selected, the chromatogram process is different. In the Calibration mode field (available if the user is assigned the right to overwrite calibration curve) define whether the user will delete the existing curve and build a new one by selecting Clear old points, or erase only the points of the defined level by selecting Clear level only, or add the calibration point to an existing curve by selecting Add. Then define the level in the case of Standard or Control Sample (level-I) sample type selection.

NOTE: If the sample type is Control sample (level-I), and that in the method a suitability test is defined with the action 'Modify calibration curve', all the calibration points of the defined level will be replaced by the value of this control sample (level-I) in case of suitability test failure.

When the archive calibration curve profile is defined in CompassCDS Configuration Manager (21 CFR11 / Audit trail / archive calibration curve), it is possible to reprocess the chromatogram with the ‘unknown’ level either with the Calibration curve used to obtain the results saved in the chromatogram (possibly old ones), or with the last saved calibration curve. Select ‘Unknown’ in the level box, and ‘chromatogram curve’ or ‘current curve’ according to the case.

If the different versions of the curve are not archived, the chromatograms are always reprocessed with the current curve.

NOTE: If a multi-channels chromatogram has to be reprocessed, repeat the operation channel by channel, by selecting the corresponding channel in the ‘Chromatogram’ field. The channel is specified in parenthesis after the chromatogram name: RUN-1(1), RUN-1(2)…

The ‘Options’ tab

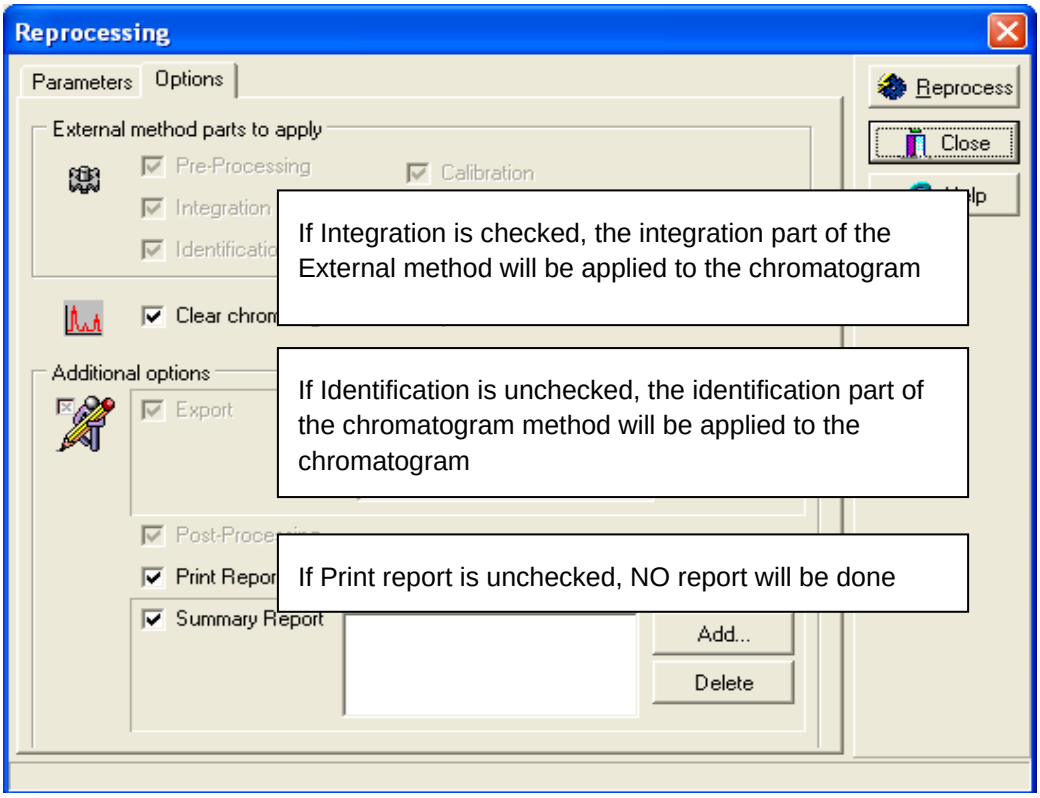
During the processing of a chromatogram, it is possible to deactivate certain processing functions. This can be useful in order to reprocess the chromatogram without printing a report for example.

When the chromatogram is reprocessed with its method, it is only possible to deactivate additional options (Export, Post processing, Print report and Summary report). It is not possible to deactivate the Preprocessing, integration, Identification, Calibration and suitability tests processes.

When the chromatogram is reprocessed with an external method, the Preprocessing, Integration, Identification, Calibration and suitability tests parts can come either from that external method (when the option is checked) or from the chromatogram method (when the option is unchecked). It is also possible to deactivate additional options (Export, Post processing, Print report and Summary report).

When the chromatogram is reprocessed, it is also possible to keep the manual operations already done on the chromatogram. To keep the manual operations, uncheck the option Clear chromatogram manual operations box.

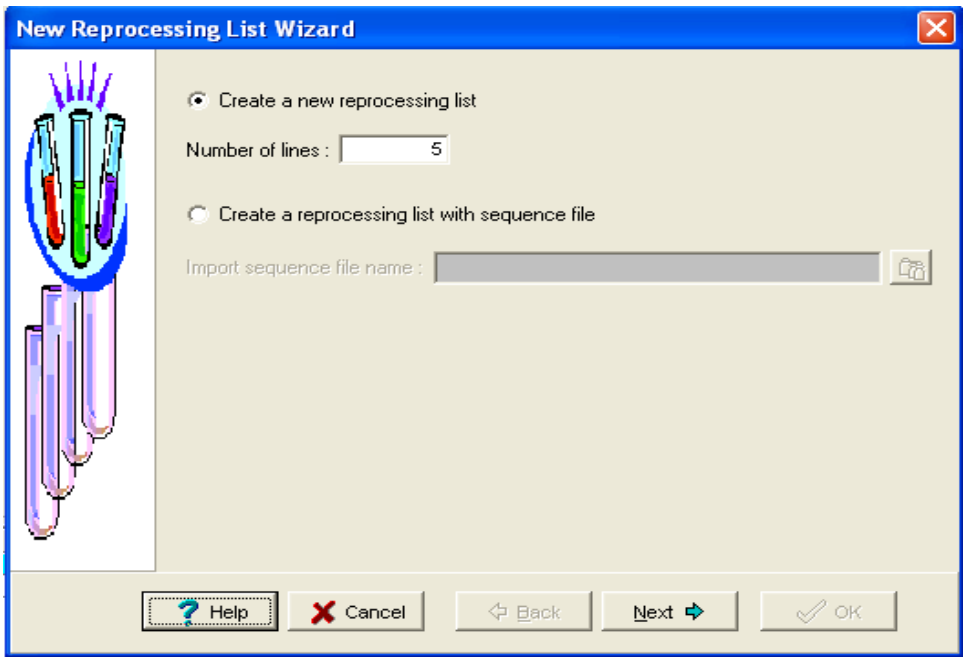
To access these options, choose the options page in the Reprocessing window.



Reprocessing Several Acquisitions: The Reprocessing List

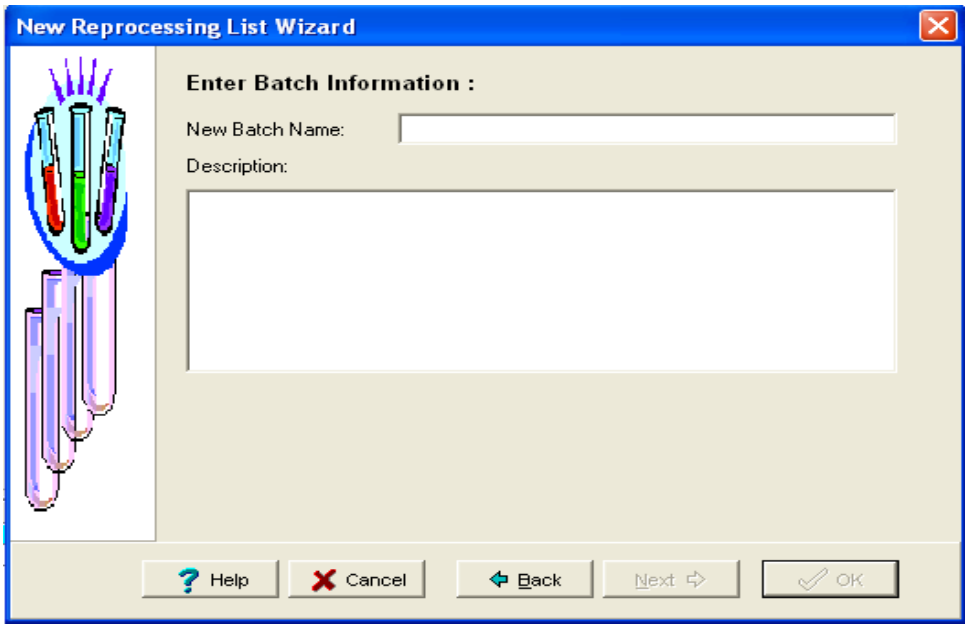
To reprocess several chromatograms rapidly, it is possible to create a reprocessing list.

Select the menu FILE / NEW / NEW REPROCESSING LIST**.** The following screen is displayed:



The user defines the number of lines of the reprocessing list, or if he wants to import chromatograms from a sequence, he has to check the second option and to select the sequence name.

Click on Next, the screen allowing the user to enter a name for the reprocessing list is displayed:



Enter a name and possibly a comment, and then click on OK. The corresponding reprocessing list is displayed.

The columns of the reprocessing list are very similar to the column of the sequence

In the “chromatogram name” column, select the name of the chromatogram(s) to be reprocessed: to open several chromatograms at the same time, press the ··· button of the first cell of this column. Then select all the chromatograms to be reprocessed with the combination of the left mouse button and the Ctrl and Shift keys. If there are more opened chromatograms than lines in the reprocessing list, lines are added at the end of the reprocessing list. Note that if selected chromatograms own several channels, one line is added by channel (by signal).

In the “chromatogram channel” column, select the chromatogram channel that should be processed: if the imported chromatogram owns 3 channels, three lines are added in the reprocessing list, with respectively the name of the detector 1, 2 and 3.

In the “method name” column, select the name of the method to apply. In the **“**method channel” one, select which channel of the method should be applied to (if the method is defined for more than one channel). Note that, when internal standards and/or user input variables are defined in the method they are imported. For example if a chromatogram has been processed with the default calibration method (area percentage), and an internal standard method is selected, the name of the internal standard(s) is imported in the ‘Istd’ column and the internal standard amount can be entered. Moreover, if a user input variable ‘A’ is defined in the chromatogram, and that this one is reprocessed with a method in which the same variable is defined, its value is kept.

In the “Method properties”, choose to apply parts either from the external method or from the chromatogram method. The Preprocessing, Integration, Identification, Calibration and suitability tests parts can come either from that external method (when the option is checked) or from the

chromatogram method (when the option is unchecked). It is also possible to deactivate additional options (Export, Post processing, Print report and Summary report).

It is also possible to keep the manual operations already done on the chromatogram. To keep the manual operations, uncheck the option Clear chromatogram manual operations box.

Values of the columns corresponding to variables saved in chromatograms (M, D, dead time, sample mass, user input, and Istd) are automatically imported from chromatograms. Nevertheless, if loading a method in which others user inputs and/or Istd are defined, the ones of the chromatogram are deleted. If common variables or Istd exist between chromatogram and method, the chromatogram values are kept.

In the ‘sample type’ column define if the sample is a standard, an unknown, a blank a control sample or a control sample (level-I).

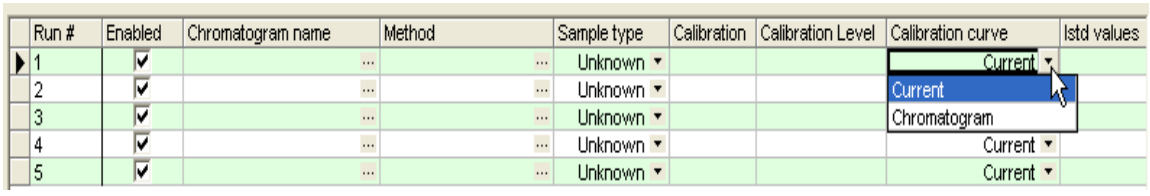
In the ‘calibration’ column, define for standard samples only, whether to keep the previous calibration points (Add), delete all the previous calibration points (Clear old points), or delete only those calibration points corresponding to the same calibration level (Clear level only). For standard samples, select the ‘calibration level’ corresponding to the quantities entered for those standards in the calibration table.

NOTE: If the sample type is Control sample (level I), and that in the method a suitability test is defined with the action ‘Modify calibration curve’, all the calibration points of the defined level will be replaced by the value of this control sample (level-I) in case of suitability test failure.

In the case of an internal standard calibration method, click on the ‘Istd values’ cell and press the ··· button, then enter the values.

Enter the User input variable values in the ‘User input’ column: click on the cell and press the ··· button, then enter the values.

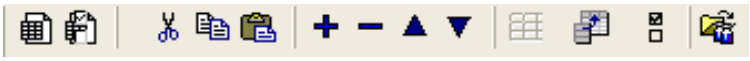
In the case that the calibration curves are archived (21 CFR11 / Audit trail / archive calibration curve), and that quantification has to be done, CompassCDS makes it possible to reprocess chromatograms either with the calibration curve used to obtain results saved in the chromatogram, or with the last archived curve. For this, precise in the ‘calibration curve’ column ‘current’ (to use the more recent curve) or ‘chromatogram’ (to use calibration curve corresponding to the saved results):



Caution: the calibration curve column only appears when the ‘Archive calibration curve’ profile has been defined in CompassCDS Configuration Manager, otherwise the chromatograms are always reprocessed with the current curve.

To work with bracketing, check the bracketing button (see page 151) to learn how to use this option in a reprocessing list).

The tool bar proposes the following options:



	This icon clears the content of all the cells of the reprocessing list
	This icon clears the unselected lines of the reprocessing list.
	This icon adds a line at the end of the reprocessing list.
	This icon deletes the selected line.
	This icon moves the selected line up.
	This icon moves the selected line down.
	This icon fills in several cells of the same column according to the content of the first one. For example, to fill in the 'Calibration level' column, select the cells to be filled in the column, then fill in the first cell with 1. Press this icon. A window appears in the workspace to define the increment between two consecutive cells. Press *OK*, and the cells are filled in. If the column contains a real value or the method, the content of the first cell is simply copied, then pasted in all others. Note that it is also possible to copy the content of a cell by selecting it, then put the mouse cursor to the left side of the cell, move the cursor down to the last cell the value must be copied, and select the fill block option in the popup menu.
	This icon permits selected columns to be hidden. Press this icon, and a window called 'Columns' appears. Unselect the columns to hide then click on OK. Be careful not to hide cells that must be filled in before the run.
	This icon allows the user to reprocess only the desired channel(s) of the listed chromatograms.
	This icon allows importation of all the chromatograms acquired in the same sequence in one step. The list of all the chromatograms of this sequence is added to the reprocessing list with the associated parameters saved in the chromatogram (M, D, dead time, mass, Istd, user input). If bracketing was defined in the imported sequence, the bracketing is kept. Of course the imported brackets can be modified afterwards.

When the reprocessing list is ready, press the start icon to run the processing. The lines are colored in green when the corresponding reprocessing has been completed. Once the entire list has been reprocessed, a message appears stating that it was "Completed".

NOTE: If defining "Blank" sample(s) in the sample type column, and use a method with a chromatogram name defined in the pre-processing part, the blank subtracted will be the one defined in the sample type column.

NOTE: It is possible to open directly a chromatogram belonging to a reprocessing list by double clicking on its name in the 'chromatogram name' column. To open several chromatograms, select the corresponding lines then choose the Open chromatogram(s) option from the context menu.

NOTE: In the case of several channels chromatogram, it is possible to uncheck the same channel(s) in all chromatograms of same structure in the total reprocessing list. In the enabled column, uncheck some channels of the first chromatogram (channel#2 in the following example):

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3

then select all the lines corresponding to the first chromatogram (for example the 3 lines in the case of 1 injectors/3 channels system):

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3

And click on the button. The pattern is applied to the entire reprocessing list:

Run #	Enabled	Chromatogram name	Chromatogram channel
1	☑	1inj-3det-1.DATA	Virtual Signal 1 #1
2	☐	1inj-3det-1.DATA	Virtual Signal 1 #2
3	☑	1inj-3det-1.DATA	Virtual Signal 1 #3
4	☑	1inj-3det-2.DATA	Virtual Signal 1 #1
5	☐	1inj-3det-2.DATA	Virtual Signal 1 #2
6	☑	1inj-3det-2.DATA	Virtual Signal 1 #3
7	☑	1inj-3det-3.DATA	Virtual Signal 1 #1
8	☐	1inj-3det-3.DATA	Virtual Signal 1 #2
9	☑	1inj-3det-3.DATA	Virtual Signal 1 #3
10	☑	1inj-3det-4.DATA	Virtual Signal 1 #1
11	☐	1inj-3det-4.DATA	Virtual Signal 1 #2
12	☑	1inj-3det-4.DATA	Virtual Signal 1 #3
13	☑	1inj-3det-5.DATA	Virtual Signal 1 #1
14	☐	1inj-3det-5.DATA	Virtual Signal 1 #2
15	☑	1inj-3det-5.DATA	Virtual Signal 1 #3

Viewing the Results

The results are saved in the chromatogram file.

To open a chromatogram, select the FILE / OPEN / OPEN CHROMATOGRAM menu, the icon or press together the Ctrl and 1 key. Select the chromatogram name(s) in the Open file window and press OK.

Integration Results Display on the Chromatogram

When the chromatogram is opened in CompassCDS its name appears in the browser. Click on Data to view the curve.

Chromatogram Scale

Once the curve is displayed in CompassCDS main screen, it is possible to magnify some parts of the chromatogram using the following two possibilities:

- Use the left mouse button: click on the top left hand corner of the area to be magnified and drag to the bottom right hand corner. Note that most of the time the width of the peaks should be emphasized more than their weight, so be careful to draw wide, but not very high rectangles.

NOTE: The chromatogram will be displayed in full scale again by clicking and dragging from any corner except the top left hand one.

- Use the popup menu (right click in the curve) options:

ZOOM IN emphasizes the curve and particularly if a zoom in has already been done, the same will be recovered.

ZOOM OUT minimizes the curve and particularly if a zoom out has already been done, the same will be recovered.

FULL SCALE returns the curve to full scale.

COPY copies the displayed chromatogram curve in order to paste it in other applications (Word, Excel, etc.).

PROPERTIES allow access to the properties to modify the display colors, view, etc...

To modify the chromatogram screen size, position the cursor between the two sections (chromatogram and method), the cursor will change to . Click and then move the limits of the display.

If the cursor is placed on the curve, the coordinates of the cursor are displayed in the status bar:

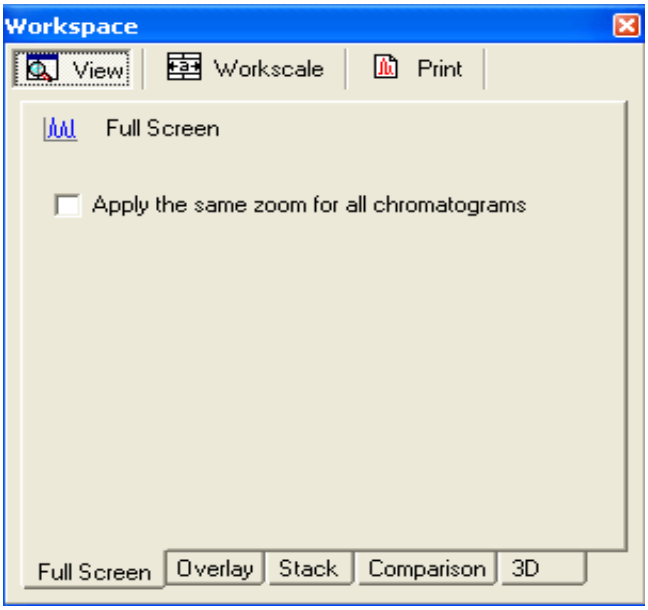
The cursor coordinates are shown after the name of the selected file.

The Workspace

The plotting of the chromatogram(s) can be modified in the workspace.

Press the icon to display the workspace.

- Select the 'View' screen to determine the display mode if several chromatograms are opened:



The following information will be displayed on each chromatogram, in the different display modes:

The X-scale and Y-scale units,

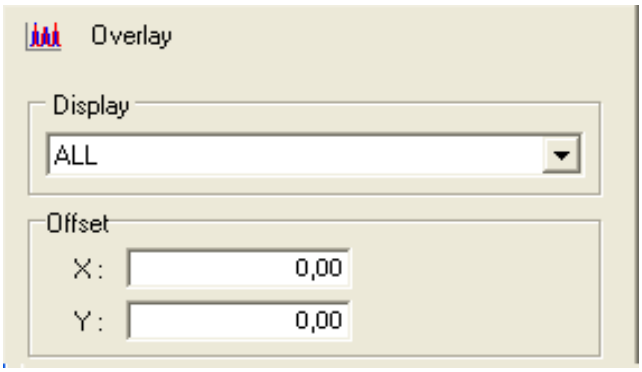
The chromatogram name with the same color as the corresponding plot,

Chromatogram annotations (peak annotations, event markers, peak markers, baselines…)

The active chromatogram name is surrounded.

FULL SCREEN: select the corresponding tab in the workspace screen or choose View / Full screen in the popup menu of the active chromatogram. In this mode, only the selected chromatogram is displayed. Click on the chromatogram name in the browser to display each curve one after the other. Check the 'Apply the same zoom for all chromatograms' option to display all the chromatograms with the same zoom.

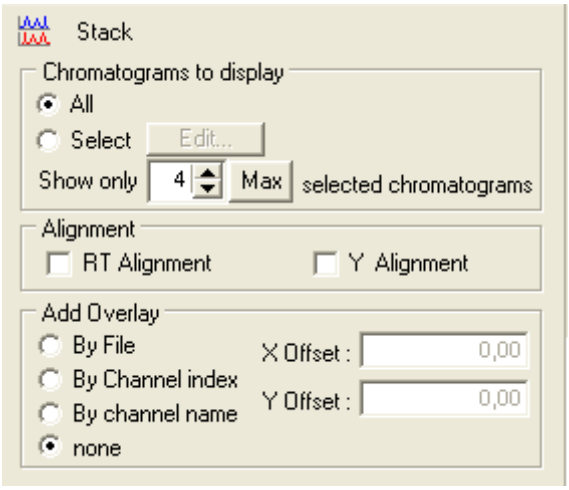
OVERLAY: Select the corresponding tab in the workspace screen or choose View / Overlay in the popup menu of the active chromatogram.



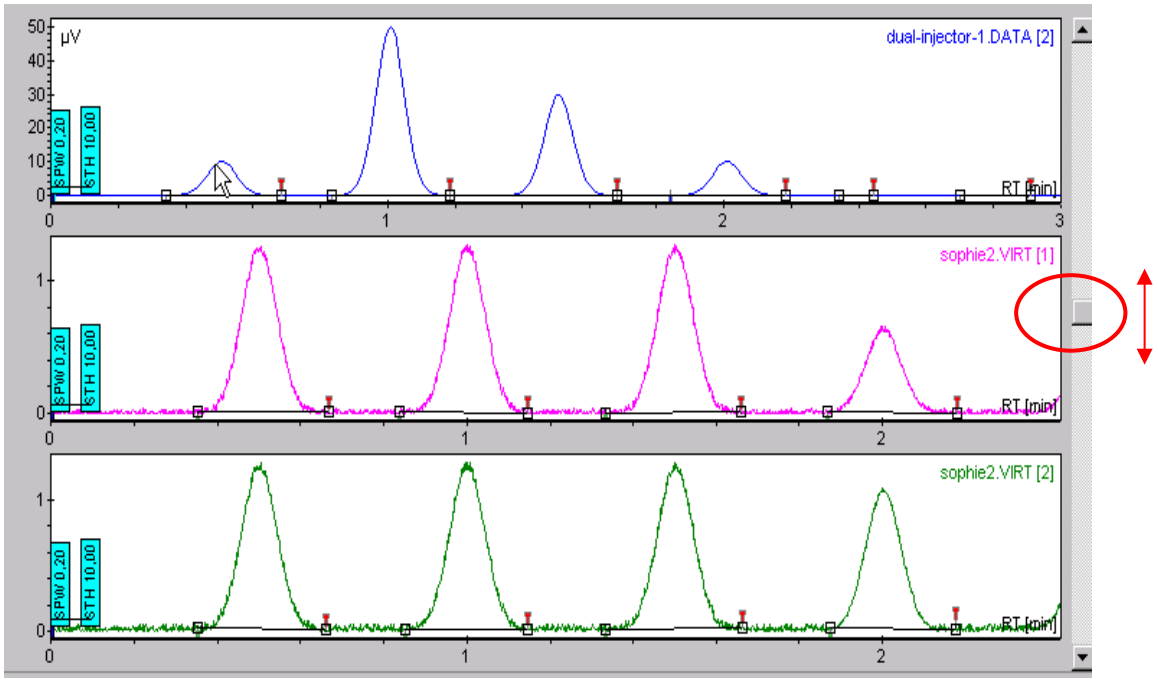
In this mode, the chromatograms are displayed in the same window. If the chromatograms are acquired on several channels (several detectors) it is possible to display only the chromatograms corresponding to the same detector. Select the required channel in the browser then choose the detector (channel) in the dropdown list. By default, ALL channels will be displayed and overlaid.

An X and/or Y offset can also be defined: the first open chromatogram will be the reference.

STACK: Select the corresponding tab in the workspace screen or choose View / Stack in the popup menu of the active chromatogram.



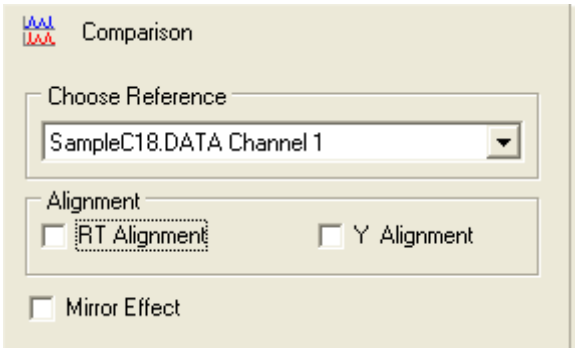
In this mode, several chromatograms are displayed in separate, stacked windows. If several chromatograms are opened, select the ones to stack in the 'Chromatogram to display' part. All the chromatograms are displayed by default, but you can also select the chromatograms to be stacked by choosing the Select option and pressing the *Edit* button. The user can also display only a few chromatograms among the selected ones, by selecting the number to display in the 'Show only X selected chromatograms' option. A scrolling bar appears which allows the display of the other selected chromatograms:



Check the RT Alignment AND/OR Y Alignment so that when zooming in on a chromatogram, or when moving it with the right mouse button, all the stacked chromatograms will be moved in the same way. To realize alignment on a defined chromatogram, select it in the browser.

If the chromatograms are acquired on several channels (several detectors) it is possible to overlay all the channels of the same chromatogram (BY FILE option) or all the chromatograms corresponding to the same channel (BY CHANNEL INDEX or CHANNEL NAME options), in the same view. ALL channels are stacked by default (no overlay): it corresponds to the NONE option.

COMPARISON: select the corresponding tab in the workspace screen or choose View / Comparison in the popup menu of the active chromatogram.

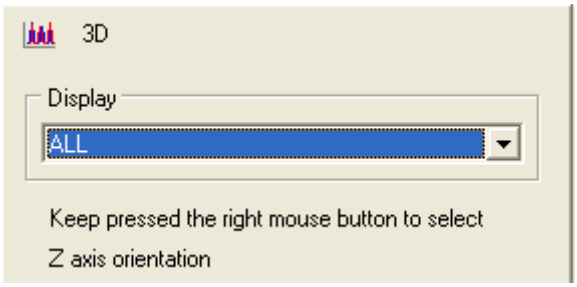


In this mode, only two chromatograms are stacked: the first one corresponds to the reference. If more than two chromatograms are opened, select the chromatogram to compare with the reference in the browser; it will be displayed in the second position, after the reference.

Check the RT Alignment AND/OR Y Alignment so that when zooming in on a chromatogram, or when moving it with the right mouse button, both chromatograms will be moved in the same way. To realize alignment on a defined chromatogram, select it in the browser.

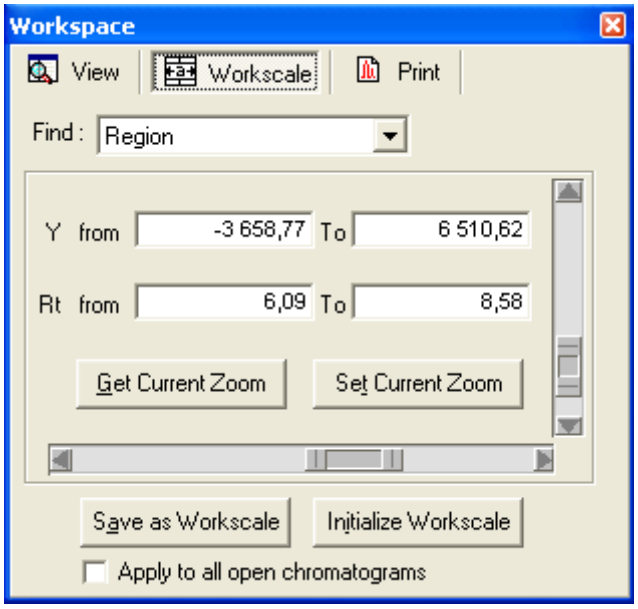
Check the *Mirror* effect option to invert the chromatogram to be compared with the reference (rotation through an angle of 180°).

3D: select the corresponding tab in the workspace screen or choose View / 3D in the popup menu of the active chromatogram.



In this mode, all the chromatograms are overlaid and can be shifted on a third axis: keep pressed the right mouse button to define the Z-axis orientation.

- Select the ‘Work scale’ tab to zoom on peaks or define manual zooms:



Select Find *Region* from the drop-down list to define manual zooms, then the limits in the Y and RT from -- to -- edit boxes can be defined. Press the Set current zoom button to apply these limits to the chromatogram.

Press the Get *current zoom* button to fill the edit boxes with chromatogram limits if the chromatogram was sized manually using the zoom in functions.

Use the scroll bars to zoom in the chromatogram: it is possible to reduce or increase the size of a bar by clicking one of its edges and dragging it. It is also possible to move them by clicking on their center and dragging them.

Select Find *Peak* from the drop-down list to zoom in on a peak: select the peak to be zoomed according to its name, index, area or height. Enter the corresponding name, index, area or height (for example ‘highest peak’) and then press the *Search* button to display the peak.

When a peak has been emphasized, use the Next and Previous buttons to view the other peaks.

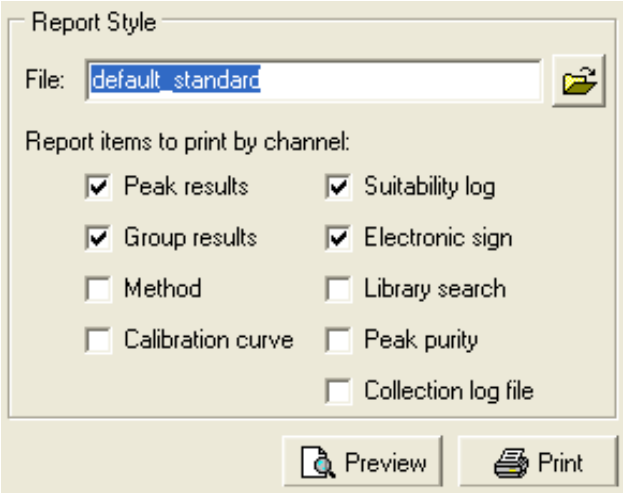
These page options can also be used to modify the working scale. The full scale is the maximum scale up permitted for zooming out. For example, if the chromatogram is composed of a huge solvent peak and many very small peaks, a full view of the solvent peak is not necessary therefore a scale to emphasize the small peaks should be defined. To set the working scale, zoom in on the chromatogram and press Save as work scale. Check the Apply to all open chromatograms box to apply this new scale to all the open chromatograms. If this work scale is customized for the channel-I of the chromatogram for instance, this customization will be applied to all channel-I of the open chromatograms only, if any.

If the working scale is not correct, press Initialize work scale to reset the working scale to the chromatogram acquisition scale.

Check the *Apply to all open chromatograms* box to reset the scale for all the open chromatograms. If this work scale is reset for the channel-I of the chromatogram for instance, this initialization will be applied to all channel-I of the open chromatograms only, if any.

NOTE: A scale defined with a manual zoom, in the WORK SCALE tab, is temporary, and is not saved in the chromatogram file when it is closed, whereas those defined and saved with the Save as work scale button will be saved in the chromatogram file.

- Select the 'Print' tab to print the results of the selected chromatograms in the same report. The following screen is displayed:



Select the report style to apply (previously built in CompassCDS Report Editor). Then select the objects to duplicate by chromatogram (one for each channel of each chromatogram). Chromatograms are printed as displayed on the screen.

Results Displayed in the Chromatogram

- **The markers:** The peak start and end are displayed with markers which can be customized. The default displayed symbols are:

Symbolizes a peak start marker: the time of the start marker is the value of the peak variable called 'Start'

- Symbolizes a peak end marker: the time of the end marker is the value of the peak variable called 'End'

Symbolizes a valley marker: this is a marker that indicates the end of a peak and the beginning of another one

Symbolizes a baseline end marker

NOTE: It is possible to select the symbol, color and markers size (Refer to page 99).

- The event annotations

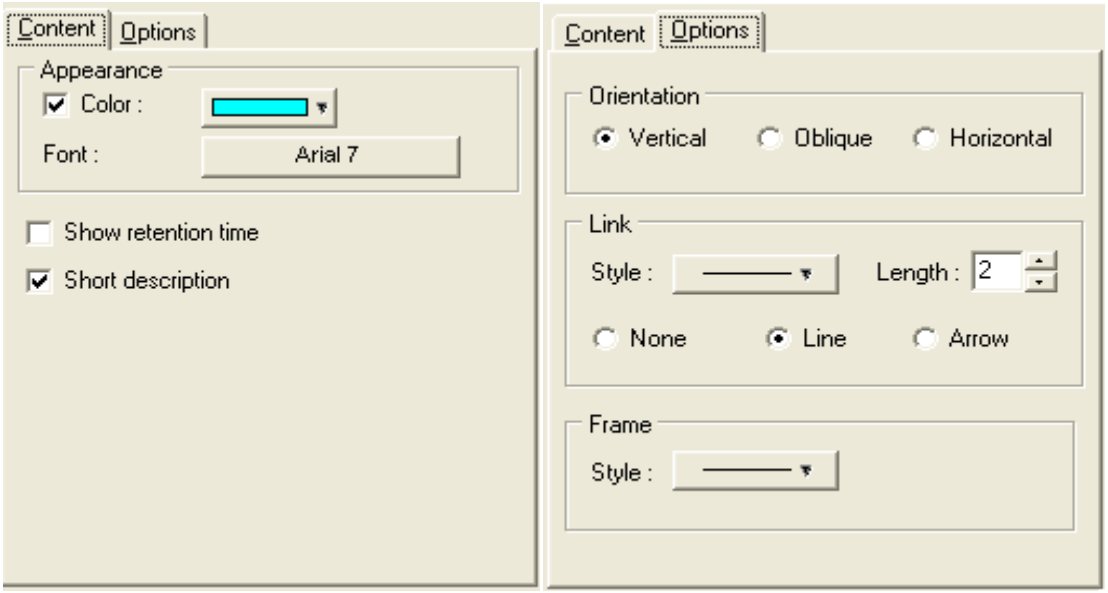
The events annotations display the integration events on the graph at the specified time.

It is possible to display or hide the integration events on the screen:

Press this button (Chromatogram annotation toolbar) to hide or show the event annotations.

Press this button (Chromatogram annotation toolbar) to hide or show the event markers.

Press this button (Display toolbar) to modify the display of event annotations. The displayed screen is divided into two sections: Content and Options.



NOTE: Those screens are also available from the Format / Chromatogram format part of the method, by selecting the Event annotations / Edit option.

In the Content tab, it is possible to modify the font and the background of the event annotations. The event description can be displayed as a code (DNP On will be displayed for Detect Negative Peaks On) by checking the 'Short description' option, or entirely by unchecking it. If Show retention time is checked in the Content page, the time when the event annotation is set, is displayed in the event annotation. For example: "1.25 DNP On" will be displayed if the Detect Negative Peaks On event was required at 1.25 minutes. Otherwise, only 'DNP On' will be displayed.

In the Options tab, define the Orientation of the annotations (Vertical, Oblique or Horizontal), the link parameters (line linking the chromatogram baseline to the event description) and eventually a frame.

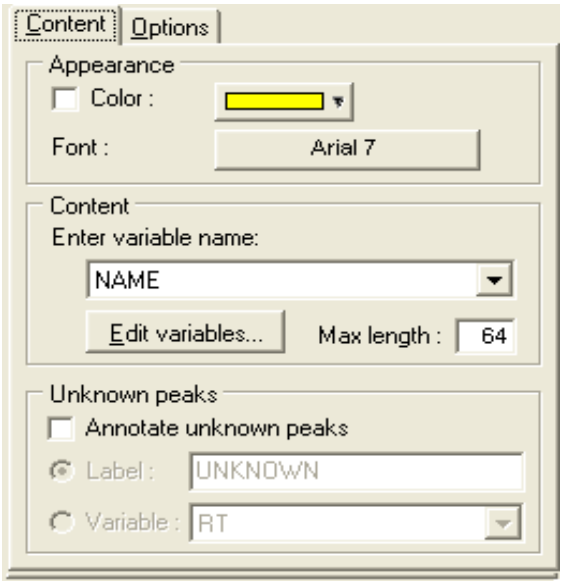
NOTE: To modify the event marker symbols, select the Properties option in the chromatogram context menu (or the Format / Chromatogram format part of the method) and select the Event markers / Customize button.

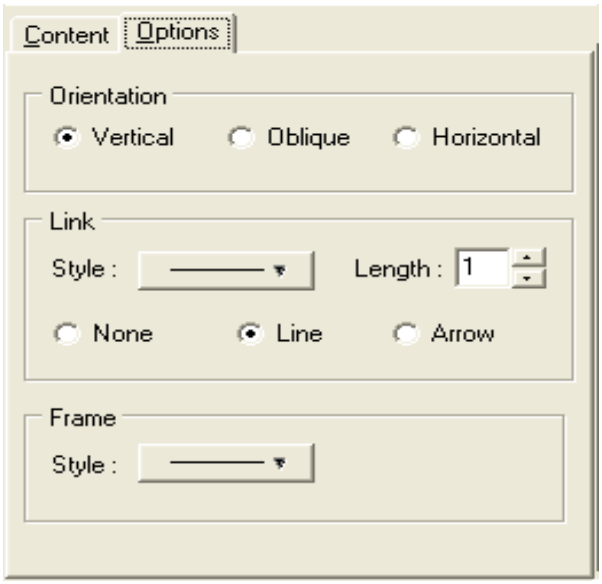
- Peak annotation

Peak annotation allows the displaying of information above each peak of the chromatogram. All the peak variables can be displayed.

Press this button (Peak annotation toolbar) to hide or show peak annotation.

Press this button (Display toolbar) to modify the display of peak annotation. The displayed screen is divided into two sections: Content and Options.





NOTE: Those screens are also available from the Format / Chromatogram format part of the method, by selecting the Peak annotations / Edit option.

In the Peak annotation window, the peak annotation display can be modified. The background color can be modified or removed. The font or orientation may also be changed.

In the Content tab, it is possible to modify the font and the background of the peak annotations. The content of the identified peak annotations can be changed and any variable defined in the variable editor (system peak variables, peak user input or peak user formula) can be displayed. To display a customized variable, grouping for example two or more variables, define a new peak user formula variable, as describe page 132).

If the annotation is too long, the user can define the number of characters to be displayed in the Max length field.

By default, no annotation is defined for unknown (non-identified) peaks. To annotate them, check the ‘Annotate unknown peaks’ option, and enter the label or choose the required variable in the drop down list.

In the Options tab, define the Orientation of the annotations (Vertical, Oblique or Horizontal), the link parameters (line linking the chromatogram baseline to the event description) and eventually a frame.

NOTE: To modify the event marker symbols, select the Properties option in the chromatogram context menu (or the Format / Chromatogram format part of the method) and select the Peak markers / Customize button.

Viewing the Peak and Group Result Calculation

The Result Tables

The results are displayed in a peak table and a group table. To view the results, click in the browser on the result section of the chromatogram channel to display.

- The Peak Table

Select the peak report item in the lower browser, and the peak table is displayed in the right panel.

Each line of the table represents a peak. When a line is selected, it is highlighted in yellow. The first and last peak markers of the corresponding peak are also highlighted in yellow in the graph.

The heading of the table columns is composed of the name and the unit of the variable. The name, the unit and the format of the variable can be modified in the variable screen. To access it, display the context menu of the desired column of the Result table and select the Edit variable X option.

At the bottom of the table, a line labeled Total is displayed in blue. The sums for all the peaks of the variables for which the total sum was required in the variable screen are displayed. The total area, height, area and height percentages, and quantities are calculated by default.

NOTE: CompassCDS can list the missing peaks in the result table, by indicating their name and theoretical retention times. The corresponding option has to be configured in the peak report format.

NOTE: CompassCDS displays areas only with positive values, i.e., if negative peaks are integrated their areas will still be positive values. To display the sign, add a column for the variable 'ISPOS' in the results table, if true is displayed the area is positive and if false is displayed the area is negative, or use the PEAKSIGN variable of the additional variables repository (see page137).

The Popup Menu:

In the peak table, press the right mouse button and a popup menu appears.

Choose ZOOM PEAK in this popup menu, and the selected peak will be highlighted in the chromatogram.

Choose COPY, and the peak table will be copied to the clipboard. Open any application (Excel is recommended), and use the local ‘Paste’ function to paste the peak report table into the application.

Choose DELETE CURRENT PEAK, and the currently selected peak is deleted (see also ‘Manual integration’).

Choose REPORT PROPERTIES to select the columns displayed in the table and modify their order.

Choose EDIT VARIABLE: XXX (in the column XXX), to edit the variable XXX and modify its format, its user name, etc.

- The Group Table

Select the group report in the browser, and the group table is displayed on the right panel.

Each line of the table represents a group. When a line is selected, it is highlighted in yellow.

The table column heading consists of the name and the unit for the variable. The name, the unit and the variable format can be modified in the variable screen. To access it, display the context menu of the desired column of the Group Result table and select the Edit variable X option.

At the bottom of the table, a line labeled, Total is displayed in blue. The sums for all the groups of the variables for which the sum total was required in the variable screen are displayed. The total area, height, area and height percentages, and quantities are calculated by default.

In the group table, press the right mouse button and a popup menu appears.

Choose COPY, and the group table will be copied into the clipboard. Open any application (Excel is recommended), and use the local ‘Paste’ function to paste the peak report table into the application.

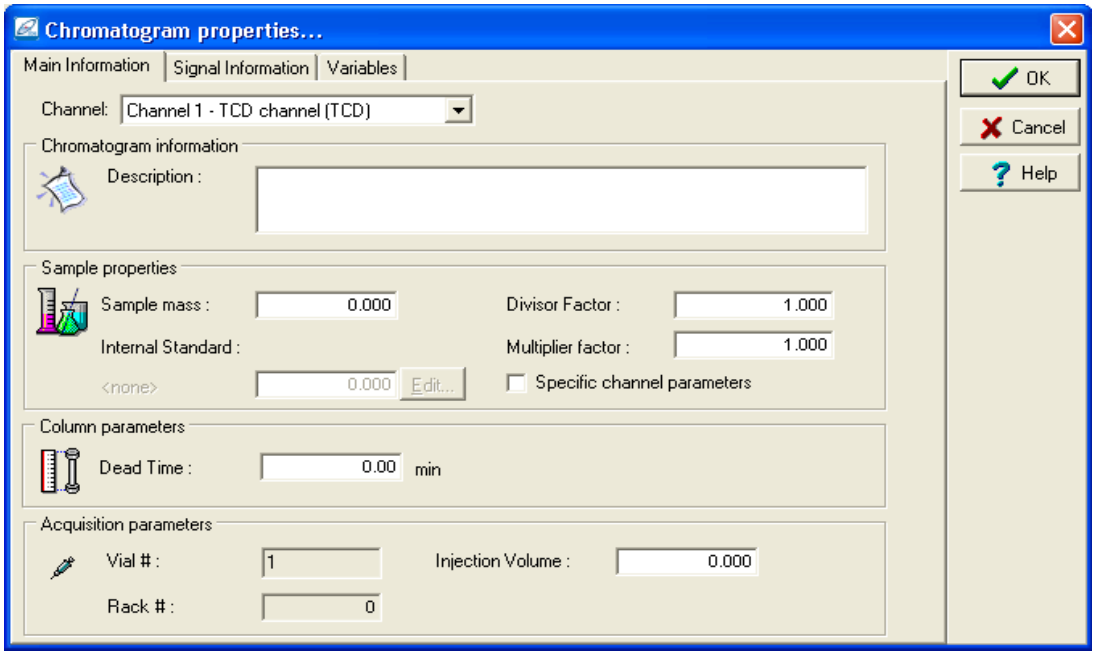
Choose REPORT PROPERTIES to select the columns displayed in the table and modify their order.

Choose EDIT VARIABLE: XXX (in the column XXX), to edit the variable XXX and modify its format, its name, etc.

NOTE: As for the peak and group result tables, the integration events, the chromatogram variable list, the calibration table, the identification peak and group tables can be copied and then pasted in Excel for example. Press the right mouse button in the corresponding table and select COPY in the popup menu.

Chromatogram Properties

To access chromatogram properties, first open a chromatogram and then select the DATA / CHROMATOGRAM PROPERTIES menu or the icon or press the F2 key. A three tab screen is displayed:



The Main information tab contains:

Chromatogram information: captured during chromatogram creation (either in the Quick Start screen or in the corresponding column of the sequence).

Sample properties: sample mass (mandatory if the result is expressed in mass% or mass ratio), divisor and multiplier (used in the quantification calculation), internal standard(s) quantity(ies), mandatory if the internal standard calibration type is selected, Specific channel parameters (except in the case of a system with one injector and one detector).

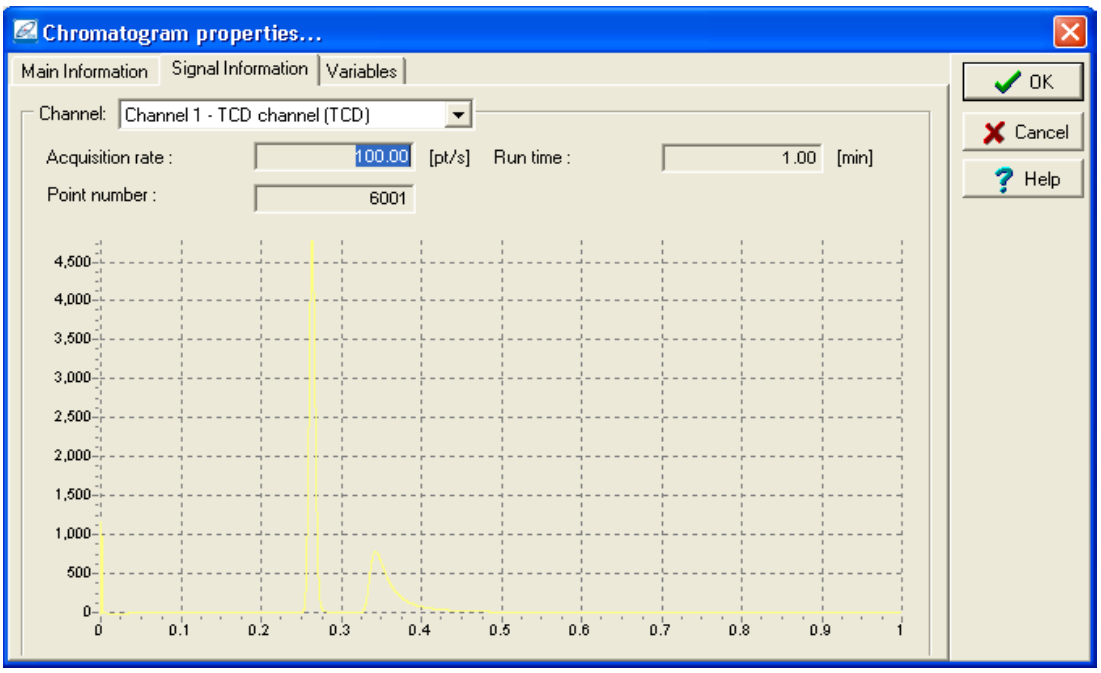
Column parameters: dead time (used for the selectivity and capacity factor calculation).

Acquisition parameters: vial and rack numbers, injection volume.

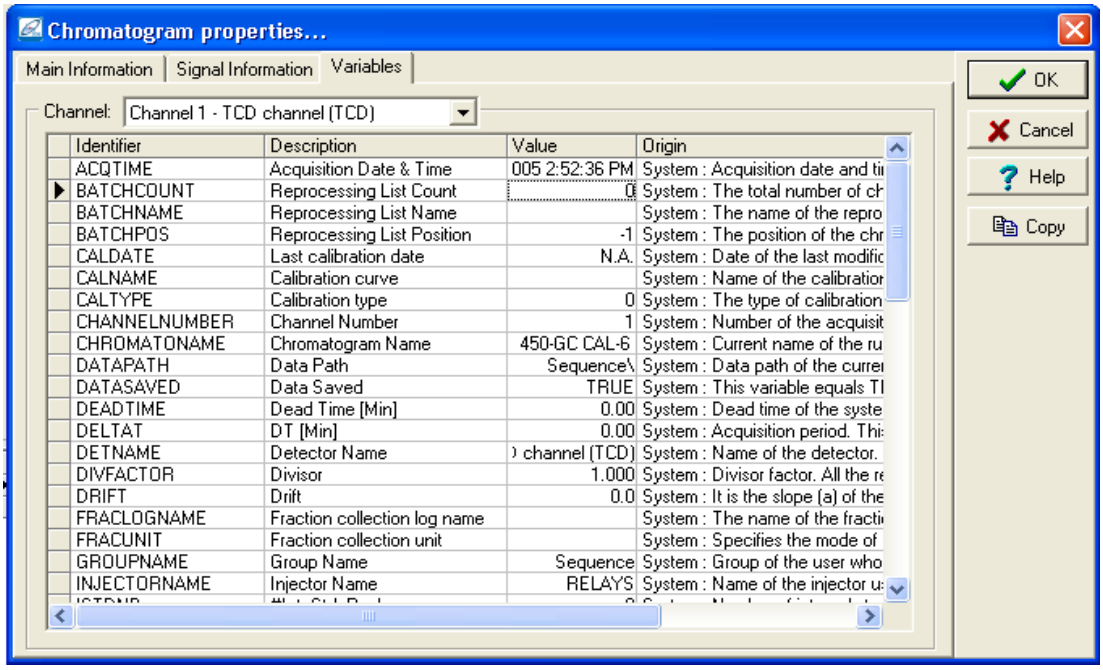
All fields except the acquisition parameters can be modified after the acquisition.

NOTE: When 'Specific channel parameters' is selected, user can select the channel name in the Channel field and complete the Sample Properties part by channel.

The Signal information tab brings together acquisition parameters: acquisition rate, run time and point number. These data are available by channel.



The Variables tab displays the value of system variables, calculated automatically for each chromatogram plus those of the global user input variables (see page 130). User input variables are displayed on a yellow background, the user can modify the values from this screen.


Chromatogram properties...
Main Information
Signal Information
Variables
OK
Cancel
Help
Copy
Channel: Channel 1 - TCD channel (TCD)
Identifier | Description | Value | Origin
ACQTIME | Acquisition Date & Time | 005 2:52:36 PM | System : Acquisition date and ti
BATCHCOUNT | Reprocessing List Count | 0 | System : The total number of ch
BATCHNAME | Reprocessing List Name | | System : The name of the repro
BATCHPOS | Reprocessing List Position | -1 | System : The position of the chr
CALDATE | Last calibration date | N.A. | System : Date of the last modific
CALNAME | Calibration curve | | System : Name of the calibratior
CALTYPE | Calibration type | 0 | System : The type of calibration
CHANNELNUMBER | Channel Number | 1 | System : Number of the acquisit
CHROMATONAME | Chromatogram Name | 450-GC CAL-6 | System : Current name of the ru
DATAPATH | Data Path | Sequence\ | System : Data path of the curre
DATASAVED | Data Saved | TRUE | System : This variable equals TI
DEADTIME | Dead Time [Min] | 0.00 | System : Dead time of the syste
DELTAT | DT [Min] | 0.00 | System : Acquisition period. This
DETNAME | Detector Name |) channel (TCD) | System : Name of the detector.
DIVFACTOR | Divisor | 1.000 | System : Divisor factor. All the re
DRIFT | Drift | 0.0 | System : It is the slope (a) of the
FRACLOGNAME | Fraction collection log name | | System : The name of the fracti
FRACUNIT | Fraction collection unit | | System : Specifies the mode of
GROUPNAME | Group Name | Sequence | System : Group of the user who
INJECTORNAME | Injector Name | RELAYS | System : Name of the injector u

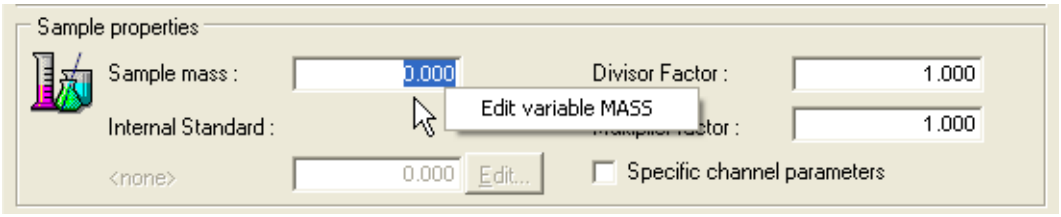
Note that it is possible to modify the format (number of significant digits, scientific format) of the following variables from this screen:

Main information tab: every variable of the ‘Sample Properties’ part and the internal standard(s) quantity (ies).

Signal Information tab: ‘Run time’ variable

Put the mouse cursor on the variable box, click on the right button, and in the popup menu select the Edit Variable XXX function, where XXX represents the variable name. The Variable Editor screen is displayed, allowing the change of selected variable format.

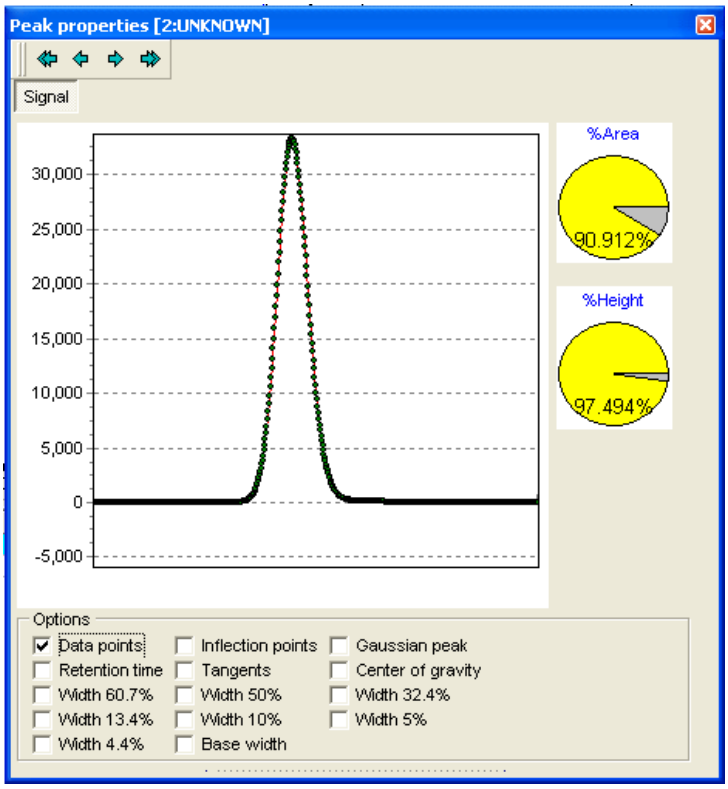
For example:



The Peak Properties

Click on to display the peak properties.

The peak properties provide an overview of the peak characteristics. Use the and arrows to scroll through the peaks.



The name of the peak is displayed as the window title. Press any of the options to view them for the selected peak. On the right of the screen, the area and height percentages of the peak are represented.

Of course, it is possible to emphasize or reduce the window size, to zoom in and out (using clicks and drags and the popup menu) within the graphics to view the details.

Click on the bar at the bottom of the screen to show or hide the options:

Printing the Results

A report can be printed automatically at the end of the acquisition. In the section of the method concerning the printed report, select a report style and the number of copies to be printed. To select a style, press the open button and choose the name of the style that will be used.

The report styles are created in CompassCDS Report Editor, the report creator. Select the FILE / NEW / NEW REPORT STYLE menu and refer to the CompassCDS Report Editor User's Guide or help file to create a report style.

To print a report manually, select the chromatogram to be printed, and press the Print icon or select the FILE / PRINT menu. A report will be printed for the chromatogram using the report style selected in the method. It is also possible to preview the report before printing using the FILE / PREVIEW menu or the Print preview icon.

If the chromatogram is not saved (displayed file different from the saved one), DATA NOT SAVED is written on the back of the report.

NOTE: The Printer Popup message can be disabled as follows: Start the Registry editor, and change HKEY_LOCAL_MACHINE\ SYSTEM\ CurrentControlSet\ Control\ Print\ Providers and set the entry NetPopup to 0. You should then reboot Windows (however stopping and restarting the print spooler will be sufficient). If the printer is on an NT server, then this setting needs to be set on the Server that controls the printed queue.

This can also be done from the Printers Control applet: Start the Printer control applet (Start - Settings - Printers); select "Server Properties" from the File menu then select the advanced tab, uncheck the "Notify when remote documents are printed". Click OK and reboot the computer.

Summary Report

The summary report provides the capability to monitor result(s) over a user-defined time interval.

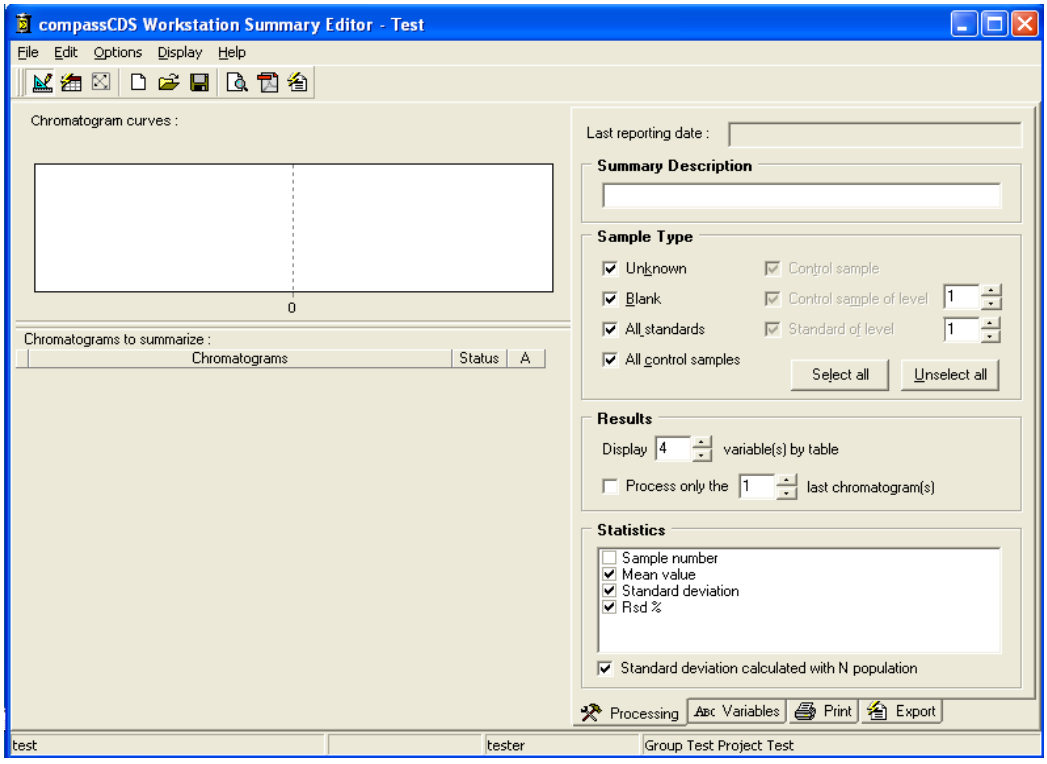
The summary report is similar to the reports created in the CompassCDS Report Editor. First, define a report style that determines what will be printed or edited and how this will be done.

Defining the Summary Report Format:

Select the FILE / NEW / NEW SUMMARY REPORT menu to access CompassCDS Summary Editor.

Processing

Select the processing tab:



On this page, select the type of chromatograms to be added automatically in the summary report and the type of statistics to be displayed in the result part.

A choice between adding Unknown, Blank, All standards or Standards of a defined level, All Control samples or only Control samples or Control sample of level is proposed. These features allow you

to filter the chromatograms to add in the summary report, when a large number of chromatograms are automatically sent.

It is possible to use only the X last added chromatograms to perform calculation, by checking the Enable the X last chromatogram(s) option where X is the desired chromatogram number.

The summary report generated consists in part of graphs and tables tracing the evolution of the variable(s). It is possible to define the variable number to display by graph/table, in the Show X variable(s) by table option.

Then define in the statistics section the calculation to realize:

Sample number: the number of chromatograms that have been added to the summary.

Mean: the mean value of the variables in the chromatograms. Note that if the variable is not calculated in a chromatogram, the mean value is not considered (i.e., its value is not considered to be zero).

Standard deviation: the standard deviation around the mean value is calculated as follows:

$s_x = \sqrt{V_x} = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n}}$ If the “standard deviation calculated with N population” option is checked

$s_x = \sqrt{V_x} = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n - 1}}$ if the option is unchecked.

Note: $\sum (x_i - \overline{x}_i)^2 = \sum ({x_i}^2) - \frac{\left(\sum (x_i)\right)^2}{n}$

Where:

x is the value of the variable in a chromatogram,

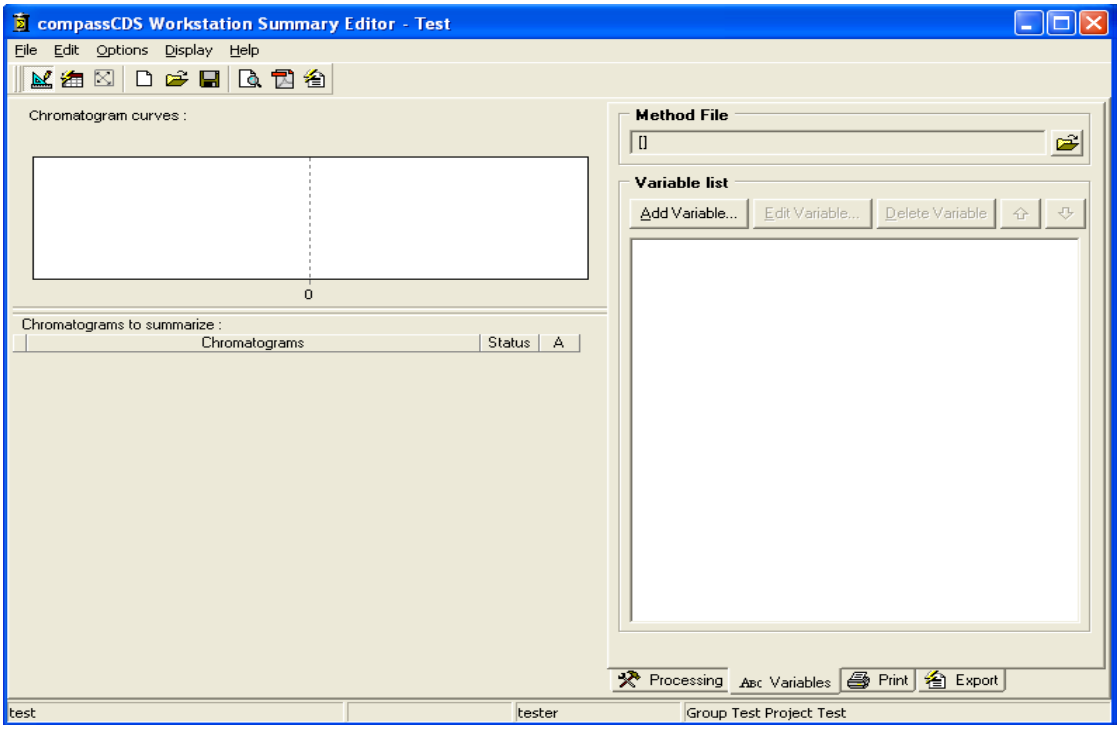
$\overline{x}$ is the mean value of the variable for all the chromatograms

n is the point number.

Residual standard deviation percentage: it is the standard deviation around the mean value divided by the mean value and multiplied by 100:

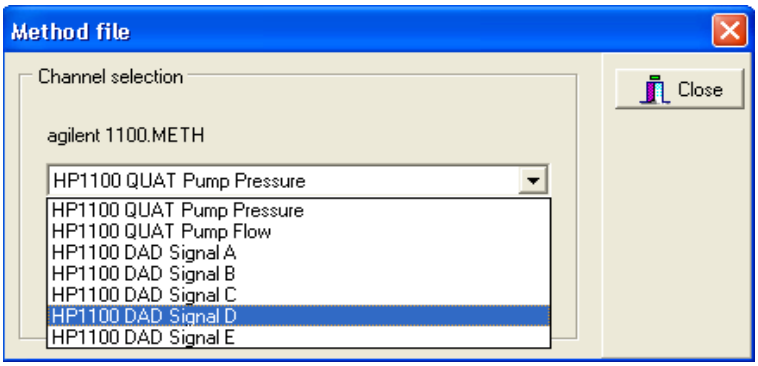
Variables

Select the Variables tab. The following screen is displayed:

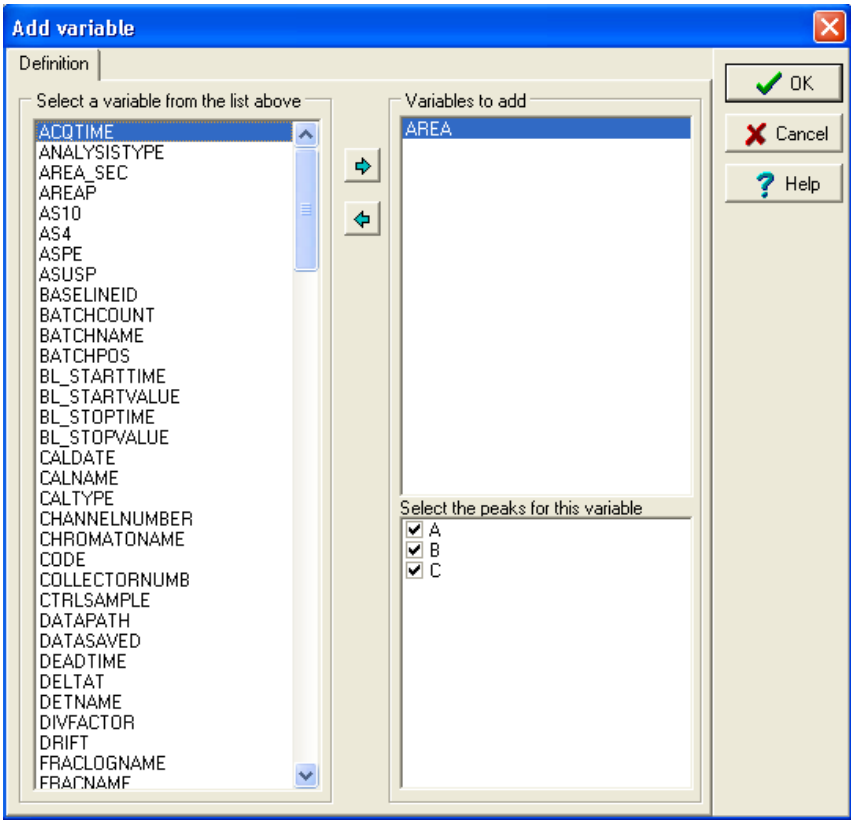


Choose the variables that will be added to the report. As the variables are defined in the method (custom variables and peak and group names), it is necessary to define a method name: Press the open ( ) icon and, in the Open file window, select the method corresponding to the type of sample to be added. This method contains the user-defined variables, as well as the names of the peaks (important if viewing a peak variable) and the format of the variables.

If the selected method contains several channels, user must specify in the following screen the channel of interest (only the variables and the peak names defined for this channel can be selected for the current summary report).



Then, in the variable list, press the left mouse button. Choose the ADD VARIABLE option. A window called ‘Add variable’ appears:

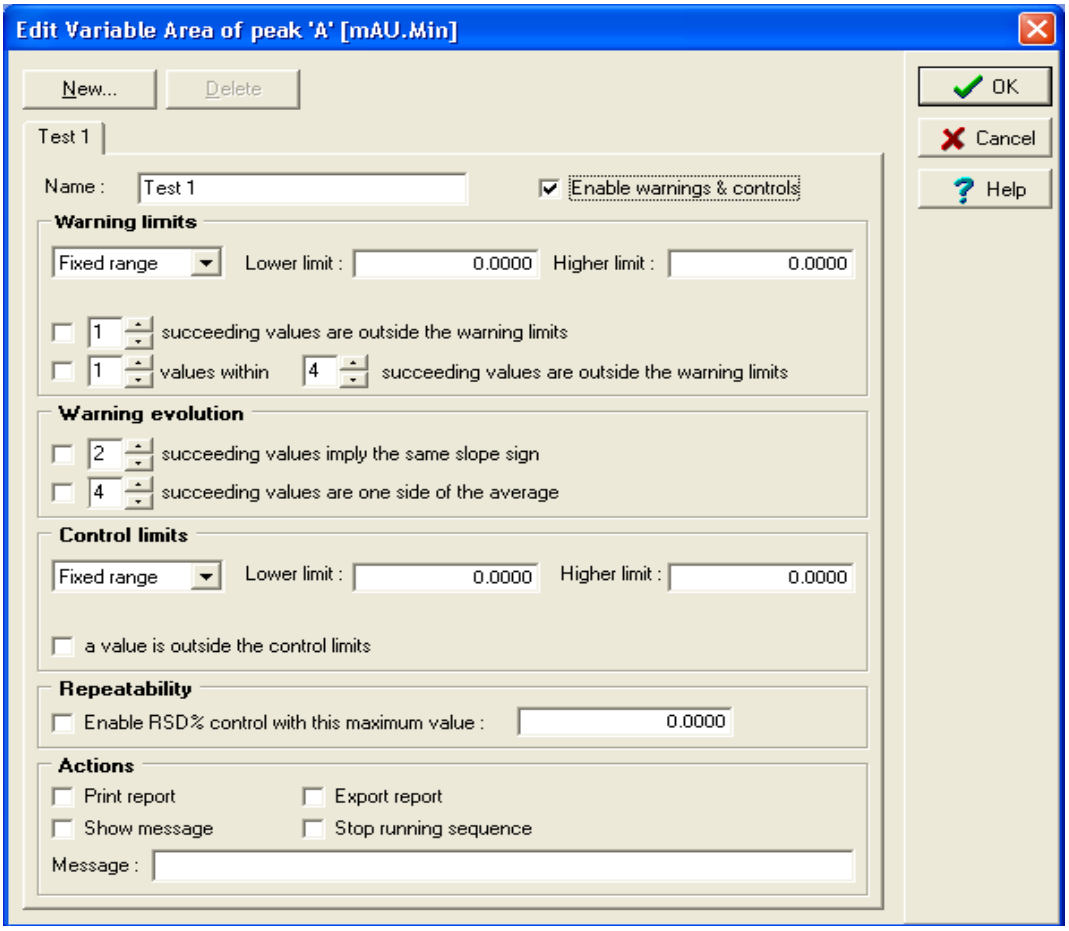


In this screen, select a variable to be added to the summary report. If the variable is a peak or a group variable, it is necessary to specify the peak(s) or group(s) concerned.

First select the name of the variable in the list, by double clicking on it or by using the arrow button. Then select the peaks concerned in the peak selection screen. By default all the existing peaks or groups are selected, the user can unselect some of them by unchecking the corresponding check box, or unselect or select all in a single action, thanks to the contextual menu.

Then validate by OK.

It is possible to define validity limits for variables added in the summary report. For that, select the variable in the ABC Variables screen, and press the button. The following screen is displayed:

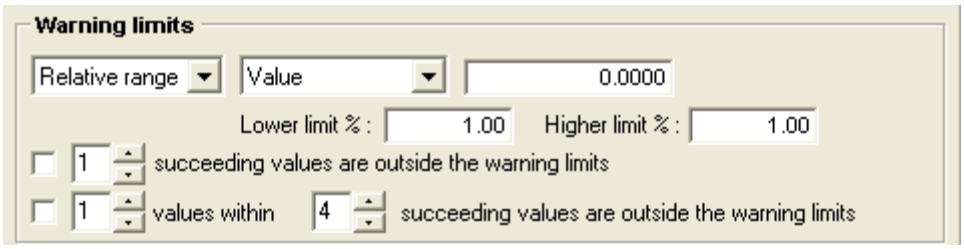


Check *Enable Warning & Control* to define limits for this variable. There are two kinds of limits: warning limits and control limits.

Warning limits are defined to advise that some problems could occur.

Control limits are limits that should never be overstepped.

Warning limits can be defined as: a fixed range, user has to define Lower and Higher limit, or as a Relative range in comparison of value, a variable or a variable mean.



Then define the conditions of the test:

- X succeeding values are outside the warning limits
- X values within Y succeeding values are outside the warning limits

User can define a Warning evolution:

- X succeeding values imply the same slope side
- X succeeding values are one side of the average

Control limits are defined in the same way as Warning limits, the same options are proposed.

Check the box Enable RSD% *control with this maximum value* and enter a value for the max %RSD.

When that option is chosen and when the %RSD is computed (see page 195), the software compares the %RSD computed for the variable to the max %RSD. A new warning is generated when the computed RSD is greater than the Max RSD%.

When the warning and controls are clearly defined, define the action to perform in the case or the test fails, among the four proposed:

Print a report, *Show message* (to define in the corresponding field), Export a report or in the case or the processed chromatogram is just acquired via a sequence, *Stop running sequence*.

It is possible to execute several tests on the same variable. For that, click on the

button. A new tab is added defining the new test conditions. You also can delete a test by activating the

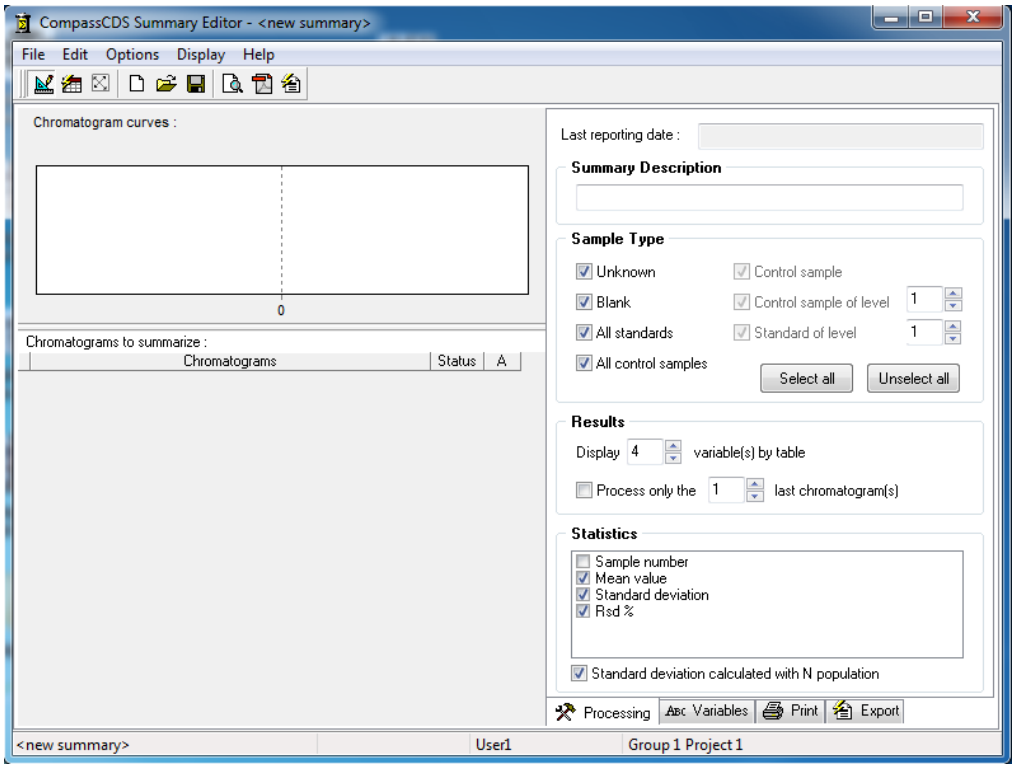
button.

When all tests are written for the selected variable, press OK. You can then select another variable and define tests.

If several variables are listed in the ABC Variable tab, you can sort them by using the up and down buttons: and , it can be useful to group all the variable of same type in the same result graphic.

Report

Select the Print tab; choose what should be printed and when the report should be printed.



First, enter a report header. This header will be printed at the top of the first page of the report.

In the Report options zone, choose what should be printed

Comments: the comments entered in the bottom of this screen,

Tables: to print the tables containing the variable values for each chromatogram,

Curves: the graphical evolution of the values,

Chromatogram list: the list of the chromatograms with their acquisition date,

Event log: the summary of all the processes done in the summary,

Warnings: the warning if some variable exceeds the limits defined in the Add variable screen,

Variable list: the list of the selected variables

Section titles: titles for all the previously selected items.

Then, in the Print report on zone, choose when the report should be printed:

At the end of every sequence or reprocessing list or at the end of every single acquisition (launched with the Quick Start).

NOTE: Report can also be printed after a warning or a control exceeding, but the print action is then defined in the variable's warning and control screen.

Note that if several summary reports are defined in different lines of the sequence or of the reprocessing list and that you have selected Sequence completed or Repro.list completed, only the summaries defined in the last line of the sequence or of the reprocessing list will be printed. To print automatically a summary report after reprocessing , select the option Repro.list completed.

NOTE: An index is associated to each chromatogram name, and this index is displayed in the array giving the statistical results instead of the entire name:

Chromatogram List

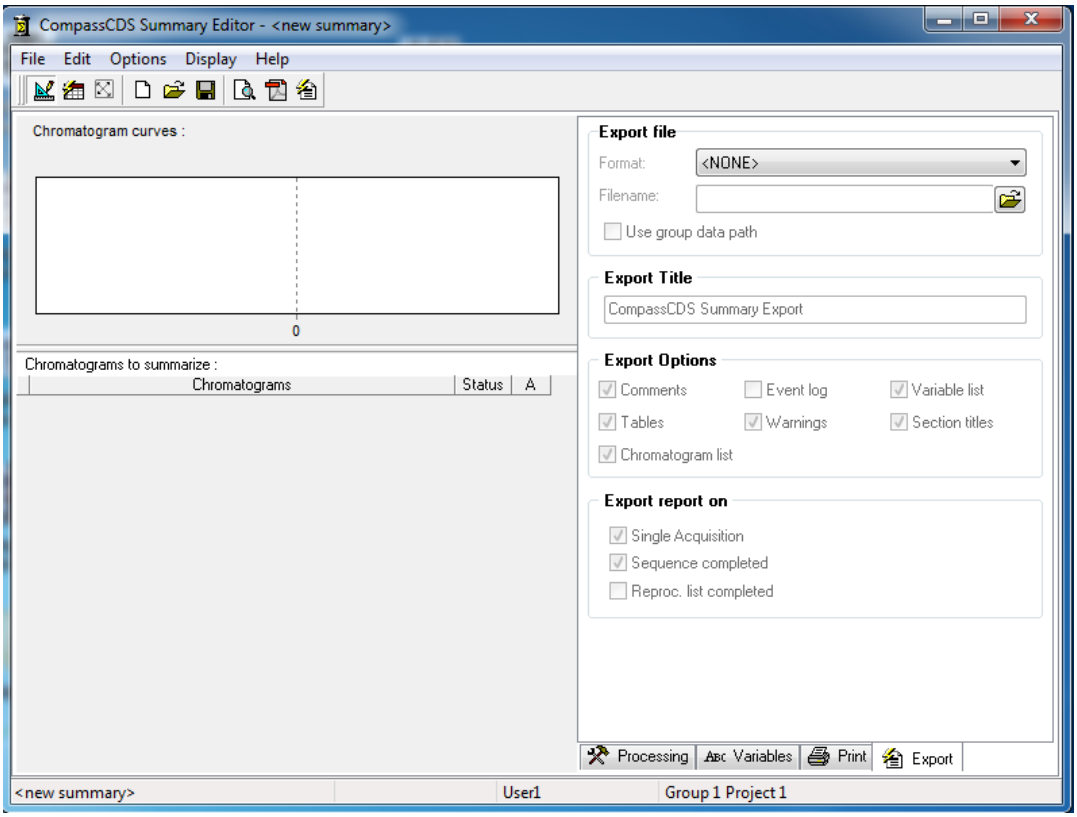
#1 - 2P-101.DATA [Channel 1]
#2 - 2P-102.DATA [Channel 1]
#3 - 2P-103.DATA [Channel 1]

Array 1

	Area/compound 1	Area/compound 2	Area/compound 3
#1			12100,1
#2			20558,4
#3			20537,0
Mean	0,0	0,0	17731,8
Std Dev (n)	0,0	0,0	3982,2
Rsd %	0,00	0,00	22,46

Export

Summary report can be automatically exported. Select the export tab.



In the Export File field, select the export file format (Excel, Word…), and specify data path and file name.

In the Export Title field, define a file name that will be displayed in the exported summary report.

In the Export options part, select which part of the report should be exported.

In the Export report on part, define when the report should be exported: at the end of the acquisition, the sequence or the reprocessing list.

Once export options have been set, save the summary.

Summary reports can be manually exported according to what has been defined in the "Export" tab, click on to do so.

How to Add Chromatograms in the Summary Report

Inside the Summary Editor:

To add chromatograms in the summary editor, select the FILE / OPEN / OPEN SUMMARY REPORT menu. In the Open file window, select the summary report to which chromatograms will be added. The summary report is opened in CompassCDS summary editor.

In the summary editor, press the right mouse button inside the panel called ‘Chromatograms to summarize’. Of course, if some chromatograms have already been added to the summary, they are listed in this zone. In the popup menu, choose ADD CHROMATOGRAM. It is also possible to use the main menu and select EDIT / ADD CHROMATOGRAM. Select the chromatograms and the channel to summarize in the Open file window and press OK.

The chromatograms are added to the summary, press the Results mode button to view the statistical results.

Automatically:

A chromatogram can be added automatically during processing in CompassCDS, after a single acquisition, after an acquisition in a sequence, or after the reprocessing of the chromatogram. In the method used to process the chromatogram, select the name of the summary report to which it should be added.

NOTE: It is possible to choose to add only a few chromatograms processed with the same method (in which a summary report is defined) in the summary report. If a chromatogram is processed and does not need to be added to the summary, uncheck the summary report options in the Processing page (see page 194).

Chromatograms Management in the Summary Report:

In the Summary Report, there is a list of the chromatograms that have been summarized (added to the summary).

These chromatograms are annotated:

	This symbol means that all the variables defined have been found in the chromatogram.
	This symbol means that a variable is missing in the chromatogram
	This symbol means that the chromatogram has not been found.

Additional information about the chromatogram is available by selecting CHROMATOGRAM INFO from the popup menu (by clicking the right mouse button) of the chromatogram list.

The popup menu helps to manage the chromatogram list. Most options are also available in the EDIT menu:

Add chromatogram: Use this menu to manually add chromatograms to the summary report.

Delete chromatogram: Use this option to remove the chromatogram from the summary report

Delete all: Use this option to remove all the chromatograms from the summary report.

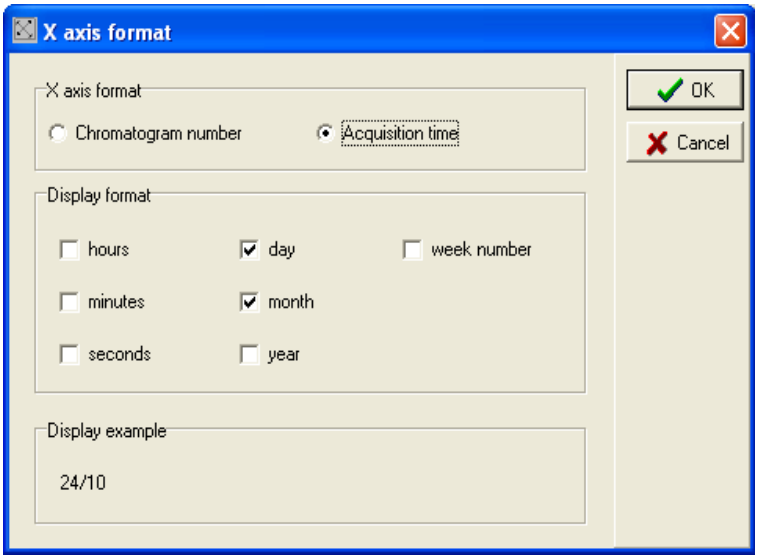
Chromatogram info: View the information about the chromatogram.

It is possible to deactivate a chromatogram for a period: its results will not be considered in the statistics. Uncheck the cell in the 'A' column: check it again to reactivate it.

Editing the Summary Report Results:

To view the summary results, press the Results Mode icon.

The tables summarizing the variable values are displayed with the corresponding graphs. To customize the X axis format, select the icon, the following screen is displayed:



By default the chromatogram number is displayed on the X axis of the graph, but the user can choose to display acquisition time and configure the time format to display.

To print the report, press the Print report icon . A preview of the report is displayed, and then presses the *Print button*. To print the report as pdf, press the Print as PDF icon:

Importing a Chromatogram (AIA format)

To import a chromatogram, copy it to the working folder and open it with the open file window as a chromatogram acquired with CompassCDS.

The chromatograms available in an AIA format are displayed as CompassCDS chromatograms in the open file window, except that their extension is .cdf instead of .data. They also contain no information or preview, and the control and acquisition sections of the method are missing.

When an imported chromatogram is opened in CompassCDS, it is displayed with CompassCDS integration and the results are calculated according to CompassCDS integration events. The peak identification parameters are not kept. Some variables concerning the acquisition are also imported: acquisition date, channel number, chromatogram name, operator name, etc.

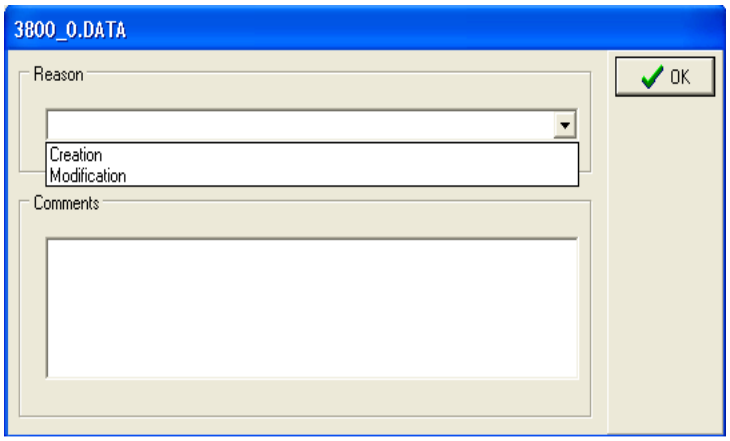
When the chromatogram is saved in CompassCDS format, a .DATA file is created.

Audit Trail

The audit trail is a tool used to trace the history of a file. Each time a chromatogram, a method, a calibration curve, a sequence, etc. is modified and saved, an archive is generated. This archive describes all the changes made, specifies the name of the user that made the change, when the change was made, and it also gives the reason and comments for change if entered by the user at the time of saving.

The audit trail is tracked only if the corresponding option is set in the profile associated with each user (CompassCDS Configuration Manager). All files or, only a few ones can have an audit trail. It must be configured in the “Audit Trail” profile.

CompassCDS offers the possibility to define or not a reason and eventually a comment for the change. If this option is selected in the CompassCDS Configuration Manager, when saving a file the following box is displayed:



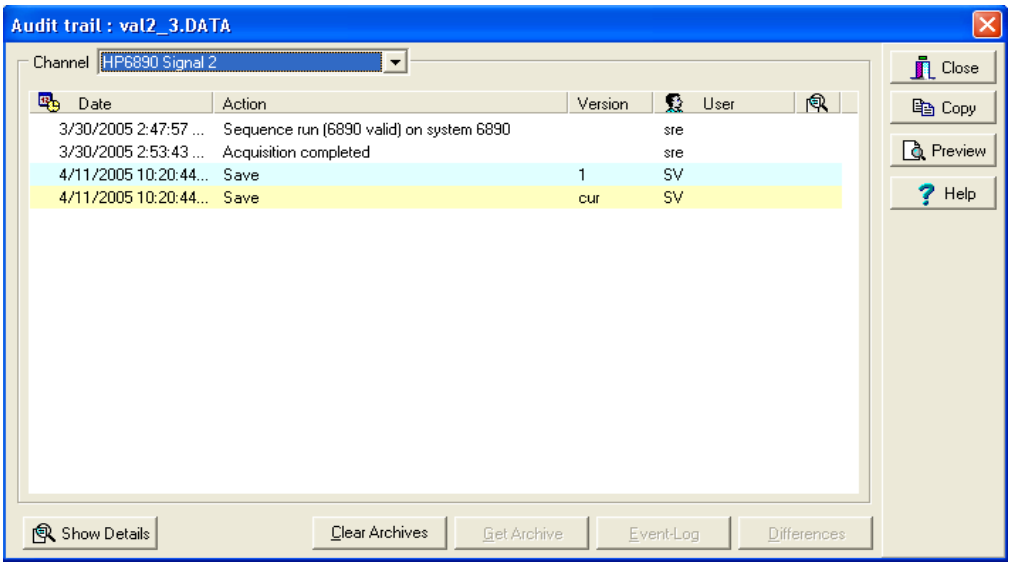
The user has to select a reason in the list given in the scrolling bar (the list is captured from the CompassCDS Configuration Manager: “Policies\Audit Trail\Configure reasons\CompassCDS

changes menu). If a mandatory comment must be entered and this is not done, then the user cannot validate and the following message appears on the screen:

The validation is possible only when a comment is entered.

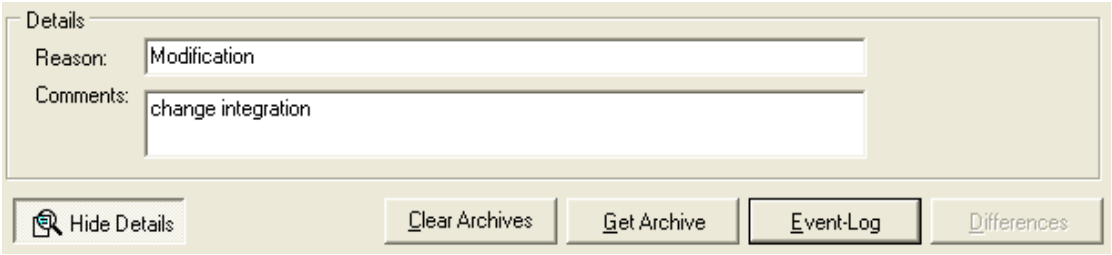
To view the audit trail of a file, open-it, then select the DISPLAY / AUDIT TRAIL menu, the AUDIT TRAIL popup menu or press the icon.

In the case of a chromatogram, the following screen is displayed:



The *audit trail* of a chromatogram or of a method are the same: Show details, Clear archives, Get archive, Event Log buttons are proposed according to the profile of the user.

This button allows the reason to be viewed and any comments entered at file saving to be viewed. Reason and comments are not mandatory, it is an optional function defined in the profiles (CompassCDS Configuration Manager). Clicking on it causes the following box to be displayed:



Clear Archives This button allows the user to clear the archives for the file. When this action is achieved a line appears in the audit trail, mentioning the operation. This button is displayed only for a user having the corresponding profile (CompassCDS Configuration Manager).

Get Archive This button allows the user to recover an old version of the file. It is, for example, possible to recover an old version of a method to process chromatograms or to use an old calibration curve version to quantify chromatograms.

Event-Log This button allows the user to view in detail the operations made. For example, each step of the treatment of a chromatogram: pre-processing, integration, identification, etc...

Differences This button is active only if two versions of the file, consecutive or not, are selected. It quickly shows the differences between the two selected versions.

NOTE: In the case of a calibration curve, the two selected versions must belong to the same calibration curve that means that two versions made before and after a “clear old points” could not be matched.

Close This button allows you to quit the Audit Trail.

Copy This button allows you to copy the Audit Trail to another application.

Preview This button allows you to view the audit trail report before printing.

Help This button allows you to reach the “On line help” (Internet Explorer has to be installed on the computer).

Save as... This button is available only if the "archive calibration curve" profile has been selected in the CompassCDS Configuration Manager. Archives are saved as calibration curve and can be used for chromatogram processing.

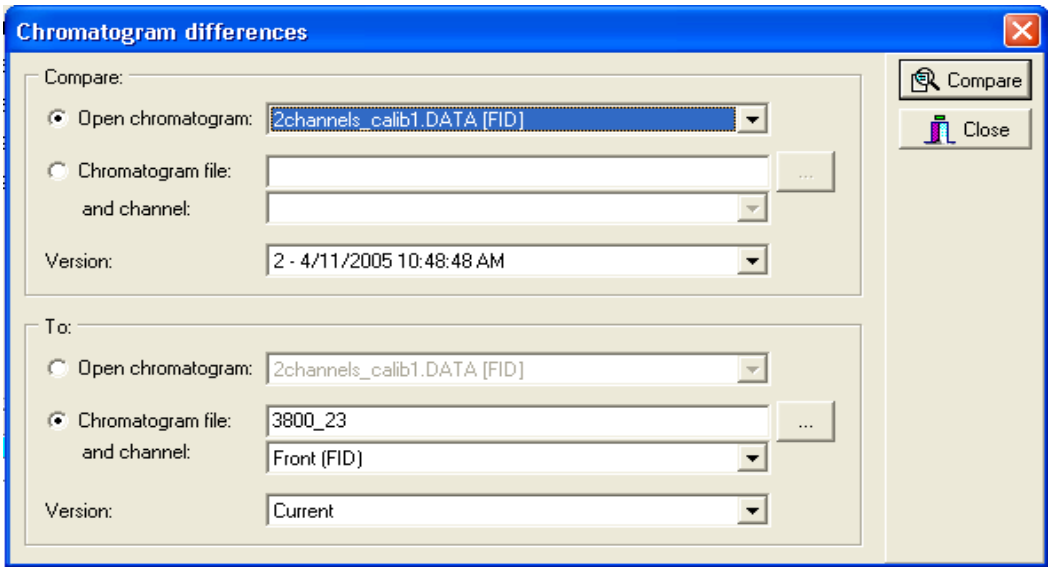
Note that for a calibration curve, the Event Log button is absent and a Save as button is present.

In the case of sequences and reprocessing lists, only the Show details, Clear archives, Get archive, and Event Log buttons are present. It is impossible to get an old version of such a file or display differences between two versions. In fact, no archives are created for these files, only a list of changes is created. Therefore, archive sequence and archive reprocessing list profile do not exist in the CompassCDS Configuration Manager.

How to Compare Two Chromatograms

CompassCDS allows you to quickly compare two chromatograms, or two archives of the same chromatogram, if the archive option was defined in the profiles in the CompassCDS Configuration Manager (“Audit Trail Profile”). The chromatograms to be compared need not necessarily to be opened.

Select the DATA / CHROMATOGRAM DIFFERENCES menu, the following screen appears.

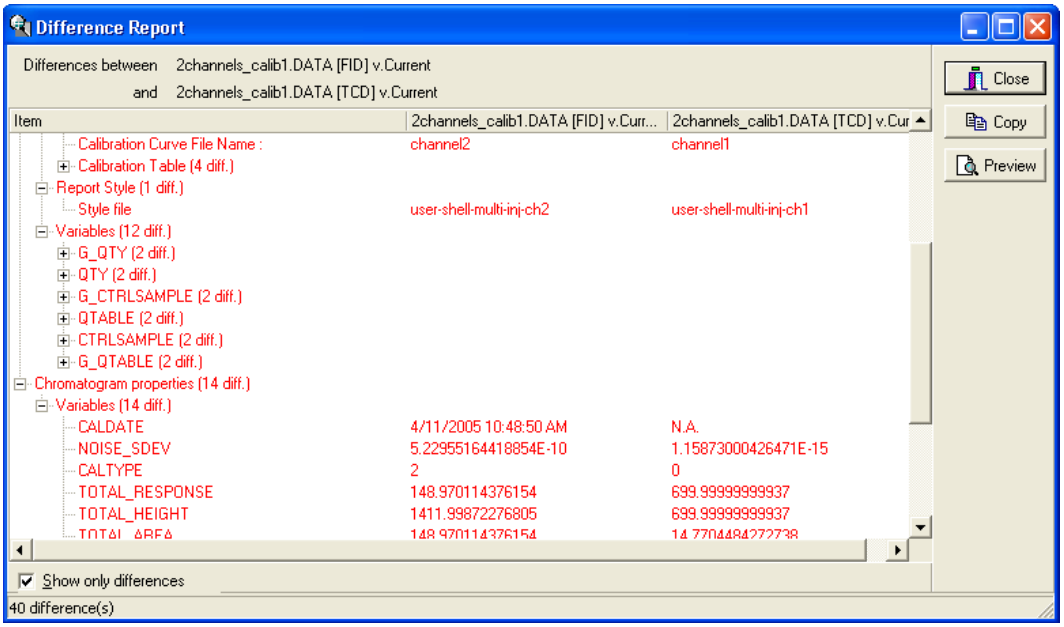


The two chromatograms to be compared are defined in the two sections of the screen.

If a chromatogram is opened and selected, its name is displayed by default in the “Open chromatogram” box. To compare a non-opened chromatogram, select its name in the “Chromatogram file” field. Define the channel to be compared in the corresponding field. In the “Version” field, select the chromatogram version to be compared, in the case where the archive profile is defined.

Once both chromatograms to be compared are defined, click on the Compare button, the differences are then displayed.

Differences only are listed if the “Show only differences” option is checked, or detailed if not. Only the differences for the chromatogram method are displayed:



User can print the difference by clicking on the

button, then on the button in the previous screen. He can also copy the differences to paste them in another application.

Electronic Signature

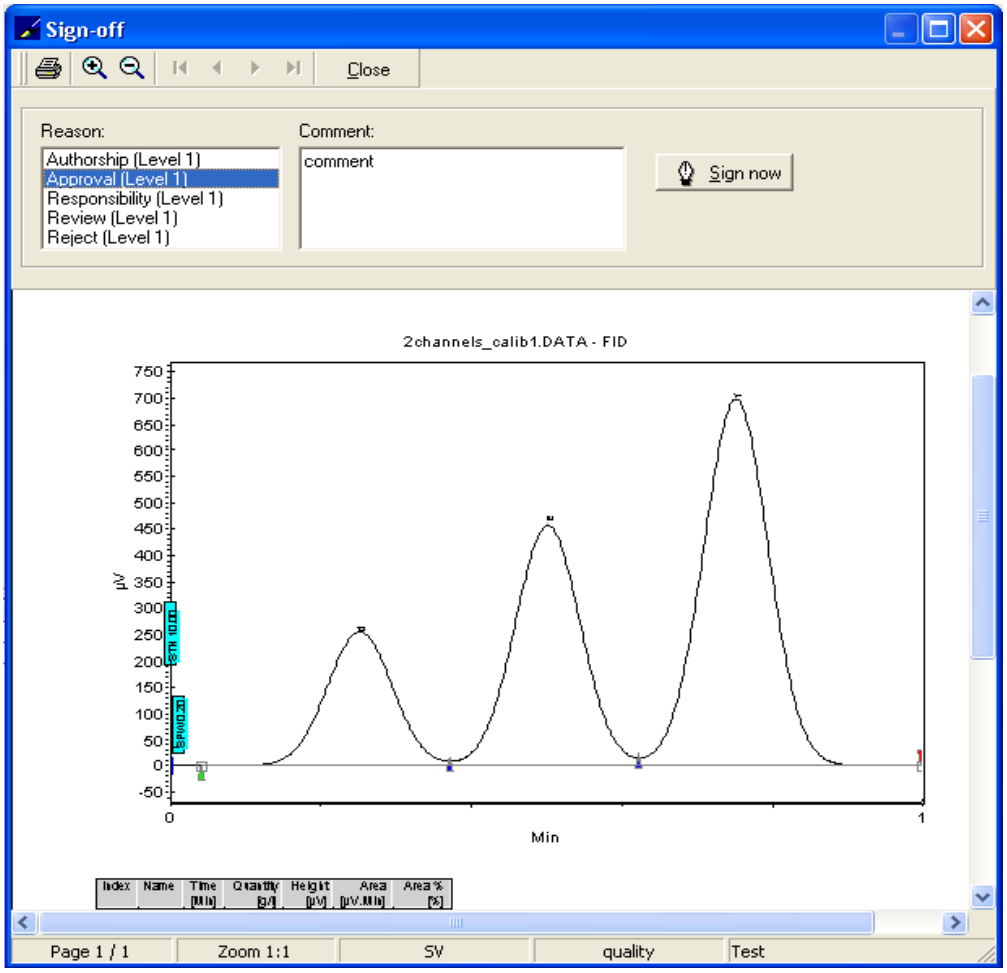
To satisfy the regulatory requirements of the FDA 21CFR11 (“rule 11”), CompassCDS offers the capability to electronically sign one or several data set for validation. Signing is executed within CompassCDS and the signature can also be printed if declared in the CompassCDS Report Editor (printing manager).

The electronic signature is accessible from CompassCDS. User can sign a single chromatogram or a batch of chromatograms.

Single Chromatogram Sign Off

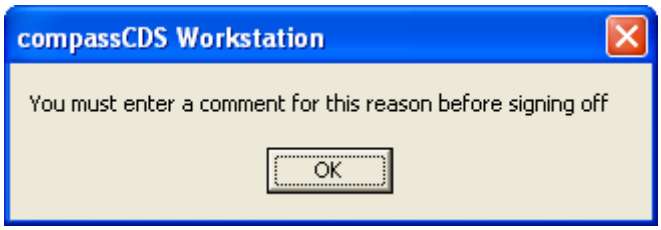
The chromatogram to be signed must be open and a report style must be associated with the chromatogram.

Click on the icon and the following screen is displayed:

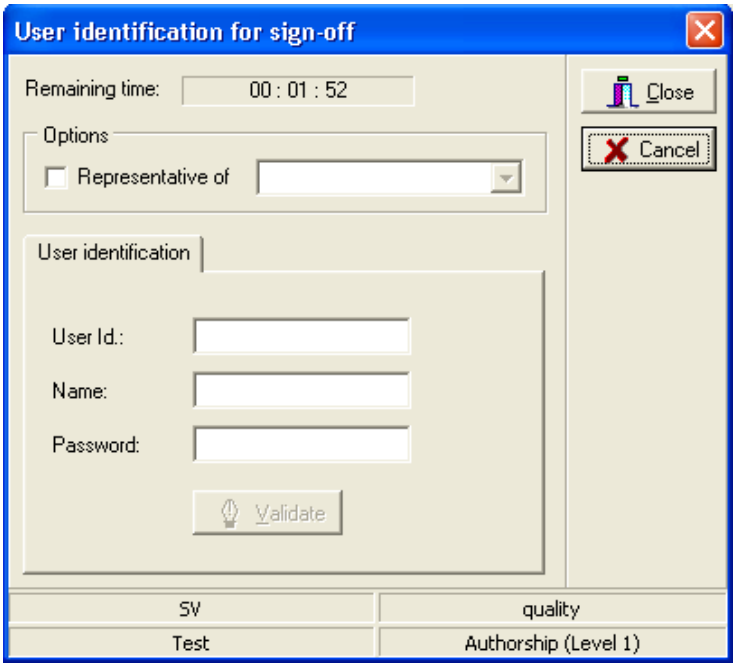


If several pages are defined, then the user has to view all the pages of the report in order to be able to sign. He must then define a reason and possibly a comment, once this is done, he can click on the button to open the sign off box.

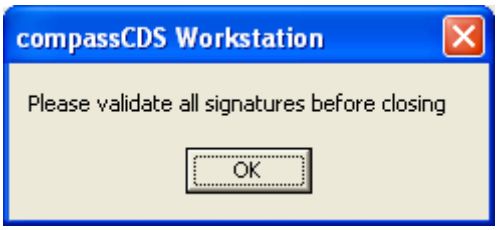
If no comment has been entered when it is mandatory, the following warning message will appear:



The following sign off window is displayed:

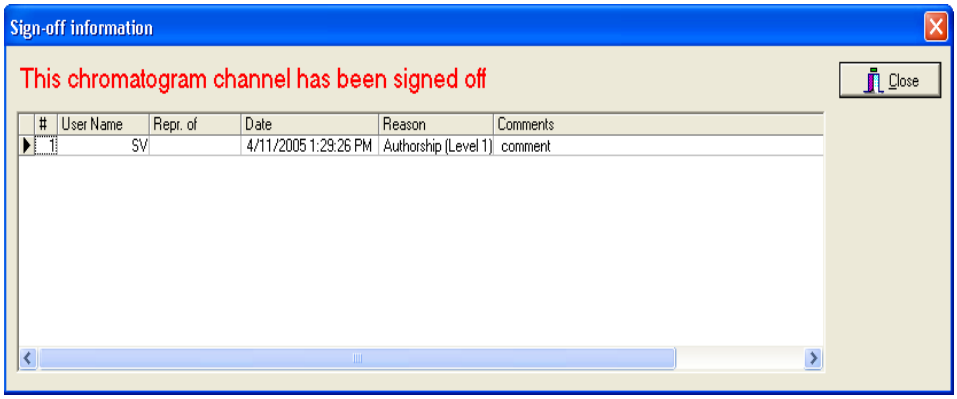


To sign, a user must identify the User Id / Password combination (defined in the CompassCDS Configuration Manager) is unique in order to formally identify the signatory. A password must have been defined; otherwise it is not possible to sign off. The user must sign within the delay defined in the CompassCDS Configuration Manager, via the POLICIES / CONFIGURATION / ELECTRONIC SIGNATURE menu (from 2 up to 10 minutes); a counter shows the remaining time and once the delay time has elapsed, the screen will close. If the user identifies within the delay period, the Validate button is active. This button must be pressed to sign off otherwise the following message will appear when closing the screen:



Several users can sign as representatives of a missing signatory. The number of representatives can be defined in the CompassCDS Configuration Manager (POLICIES / CONFIGURATION / ELECTRONIC SIGNATURE menu): at least two different users can sign as representatives of a missing one. All the representatives must also sign within the delay defined in the CompassCDS Configuration Manager, while the Validate button is active. The name of the missing signatory is selected from the list in the scrolling bar, where the names of all users defined in the project is shown.

To view the sign off for a file, open it and then click on the icon. The following screen is displayed:


Sign-off information
This chromatogram channel has been signed off
Close
User Name Repr. of Date Reason Comments
1 SV 4/11/2005 1:29:26 PM Authorship (Level 1) comment

The name of the signatory, if applicable the name of the representative signatory, the date of the sign off, the reason and any comments are displayed.

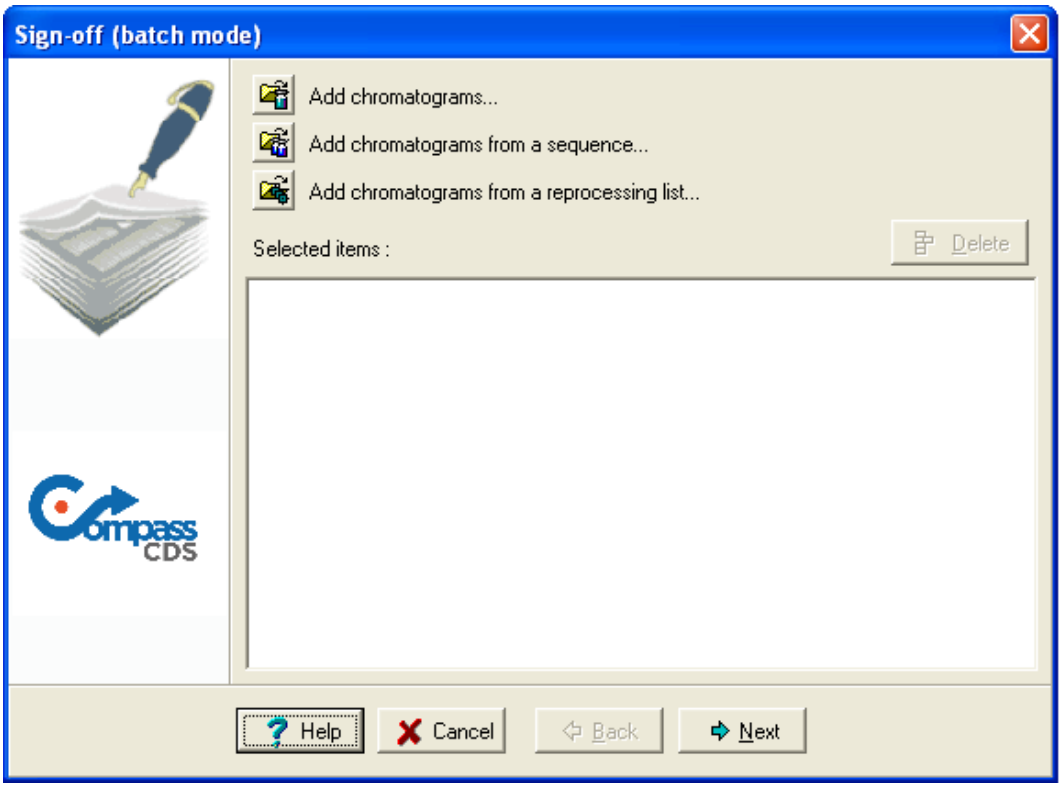
NOTE: If a change is made to the chromatogram file (integration, identification, quantification, etc.) and saved after the sign off, the sign off is deleted and must be repeated if necessary.

Chromatogram Batch Sign Off

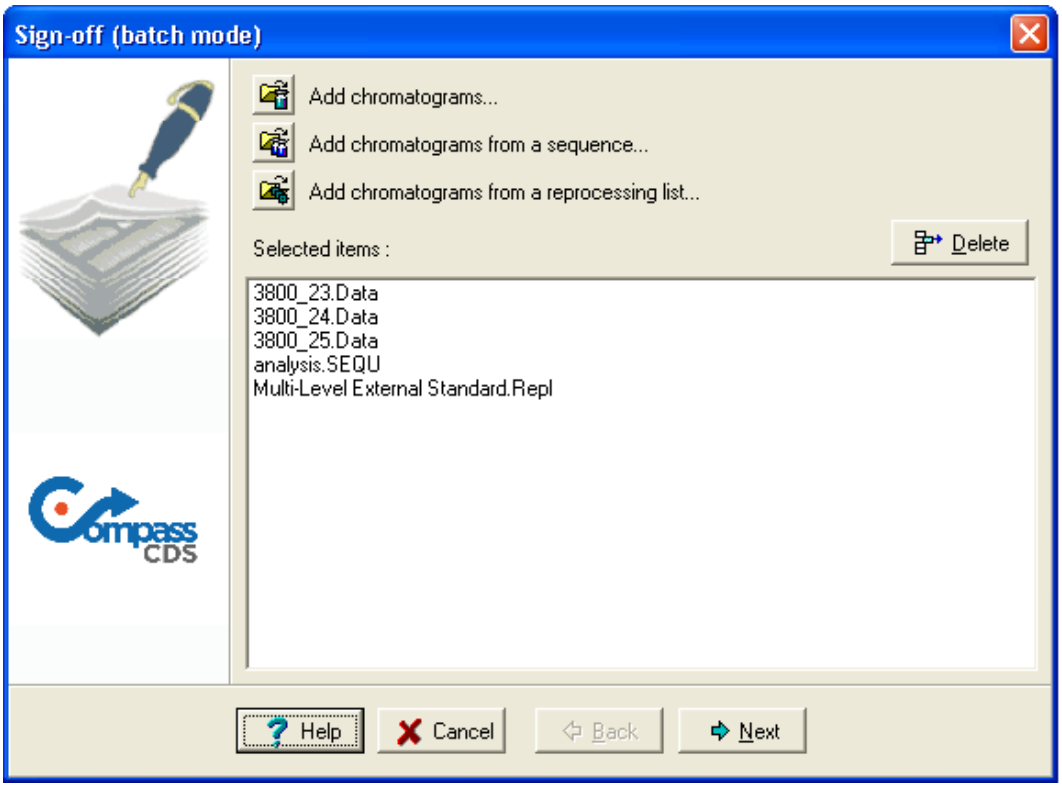
Signature of chromatograms one by one

An option allows the user to sign several chromatograms in batch. A report must be associated to each chromatogram.

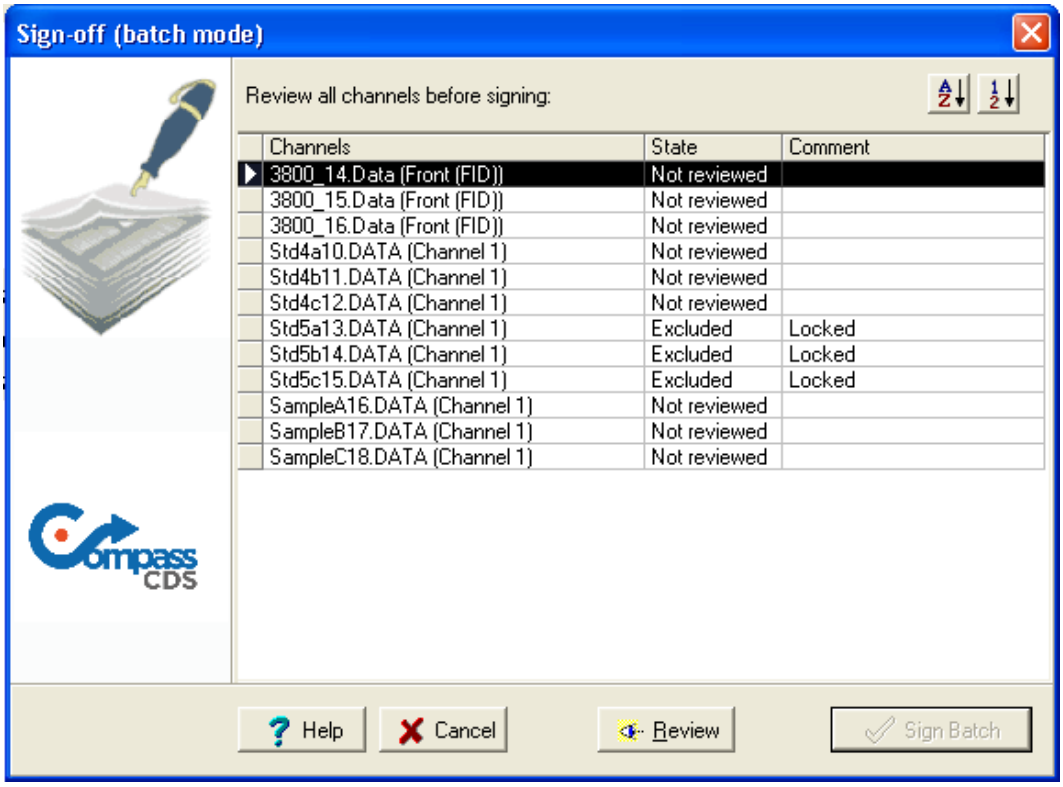
Select the icon. The following screen is displayed:



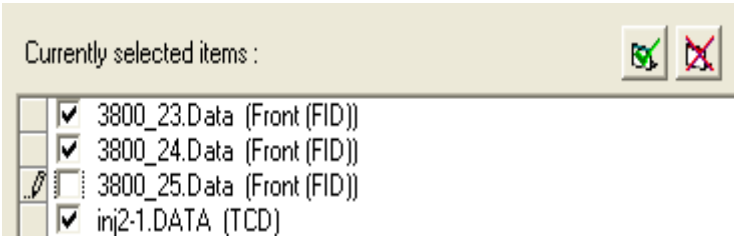
User can add chromatograms by selecting the Add chromatograms option, or all the chromatograms acquired within a sequence by selecting the Add chromatograms from a sequence, or all the chromatograms contained in a reprocessing list by selecting the Add chromatograms from a reprocessing list. The selected objects (chromatograms, sequences or reprocessing lists) are then listed in the Selected items field.



Then click on NEXT. The screen listing the chromatograms to sign is displayed:



The chromatograms corresponding to the previous selection are listed in this screen, one line is added by channel. The user can remove some chromatograms from the list by un-checking the associated box. To check or uncheck several chromatograms in a single action, you can use the Shift and Ctrl keys, or extend the selection of the lines:

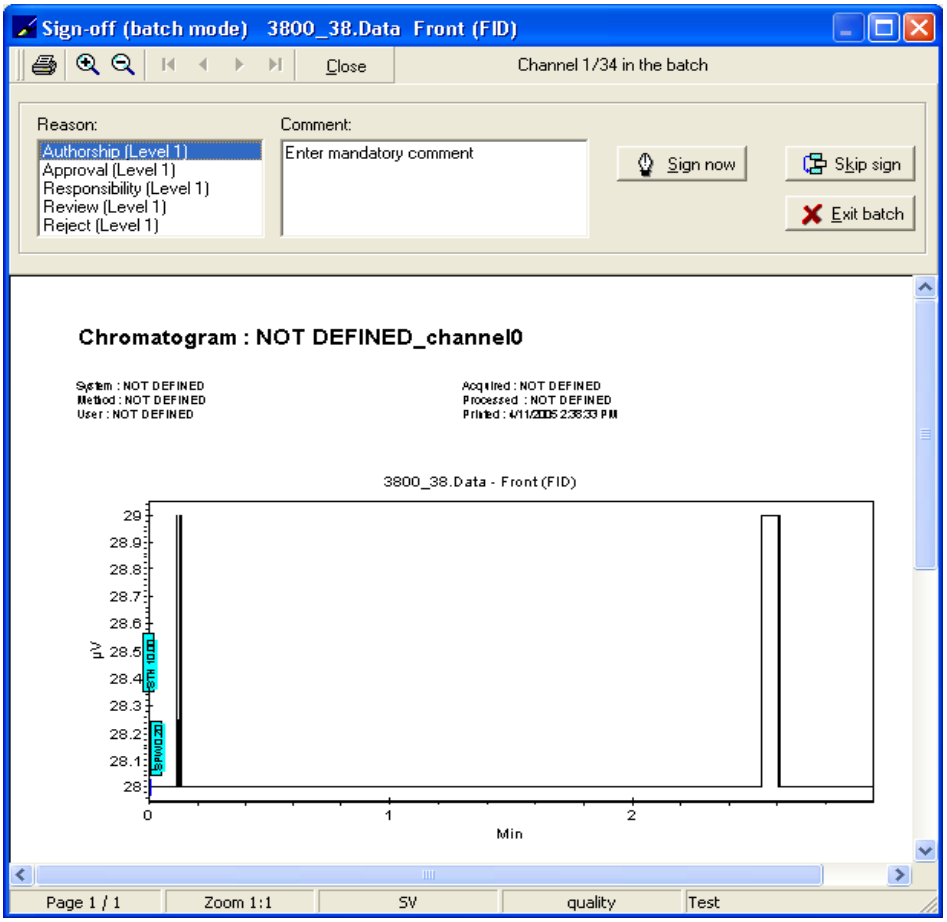


Then click on the Check selection icon or Uncheck selection icon .

It is also possible to sort the chromatograms either by name ( ) or by channel ( ), to make the selection easier.

Once the chromatograms to sign have been selected, click on the Begin review button.

The following screen is displayed:



The report of the first selected chromatogram is displayed. The user must read all the pages of the report to be authorized to sign it. If a mandatory comment is required, the user must enter it in the corresponding field before pressing the button.

A message indicates in the top of the screen, the position of the current chromatogram in the batch: means that the user signs the first chromatogram on a list of height.

If pressing the button, the following screen is displayed:

The user must enter his User Id and password in the corresponding fields, click on Validate to confirm the signature, then on the Close button to exit this screen.

NOTE: Some users can sign as representative of a user, as in the single chromatogram process (see p 62). In that case, all the representative users must sign each chromatogram together.

The screen displaying the report of the following chromatogram is then displayed; the user must read the report in total, and then press the Sign now button. The same screen as the previous one is displayed again, but the User Id is pre-defined, to avoid the user to enter it again. The user has to just enter his password for identification, and then validate the signature.

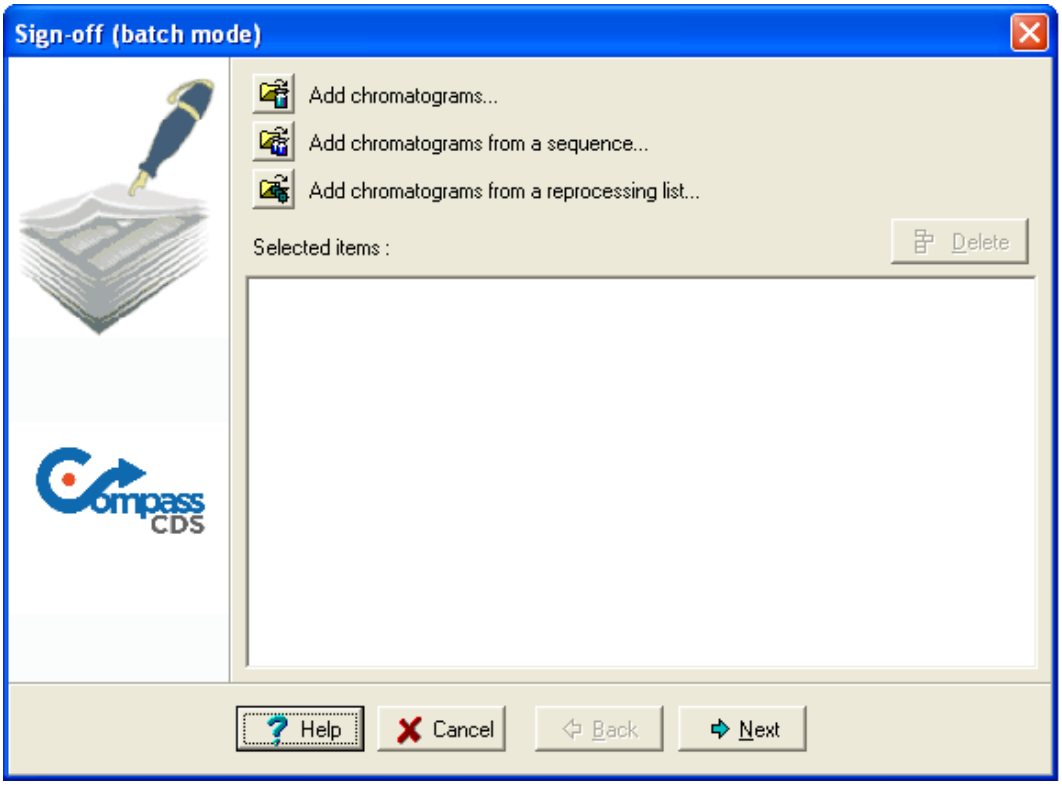
The operation has to be reproduced for each chromatogram to sign.

If the user does not want to sign one of the selected chromatogram, he can cancel the signature by pressing the Skip sign button in the report edition screen. The following chromatogram of the list is then proposed for signature. To stop the batch sign off process, press the Exit batch button, the batch sign of wizard is closed, the chromatogram selection is lost. In that case, all the already signed chromatograms keep their signature.

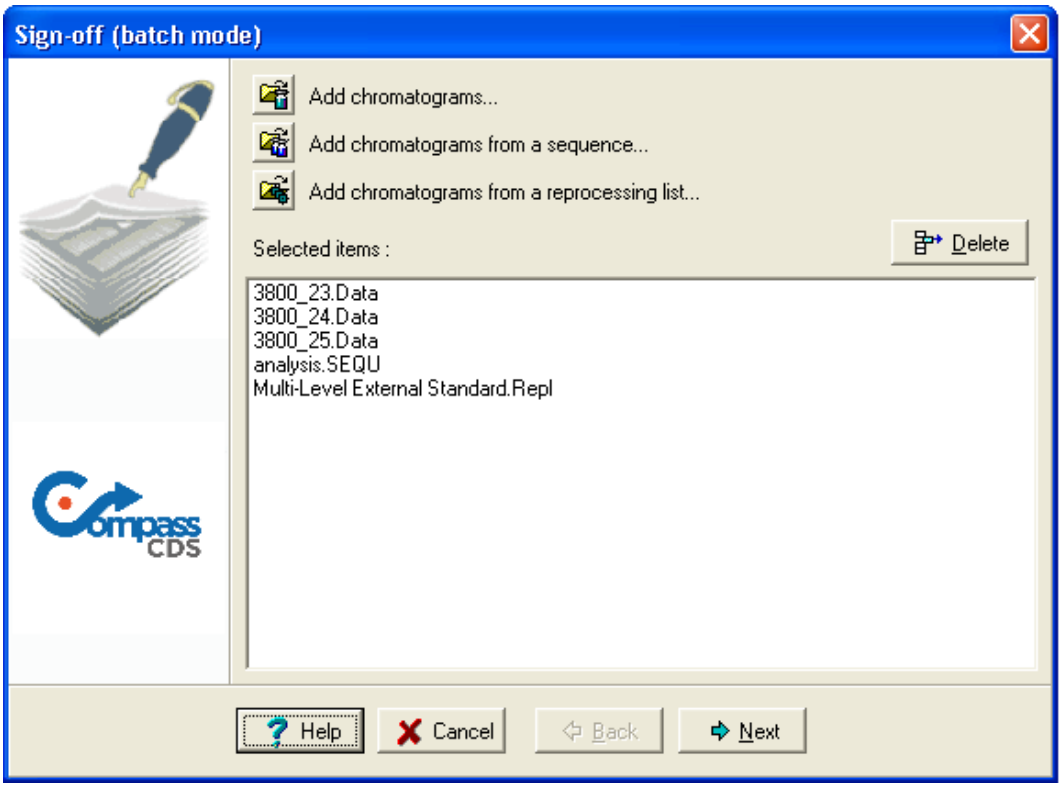
Signature of Chromatograms in One Batch

CompassCDS proposes an option allowing the user to sign several chromatograms in one batch, by defining only a single time its name, password, reason and comments. To use this function, the connected user must be assigned the '21CFR11-user / Electronic signature / Allow batch sign at once' right in the CompassCDS Configuration manager.

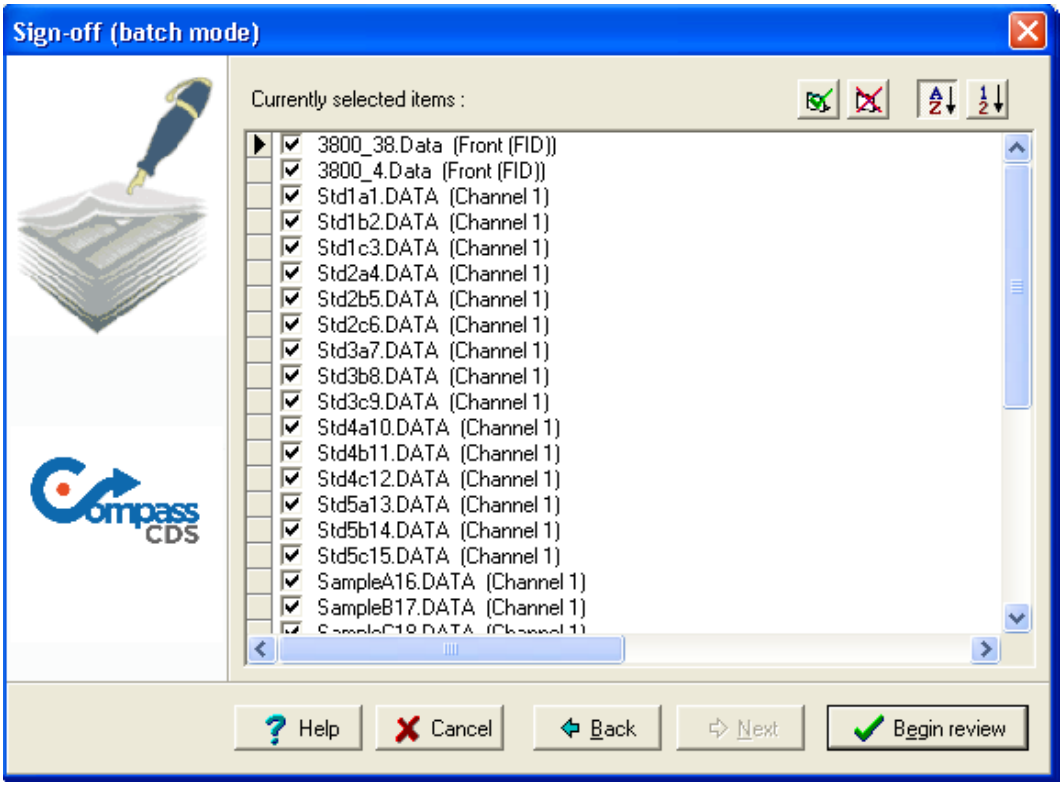
The user has to select the chromatograms he wants to sign in one batch by selecting the icon. The following screen is displayed:



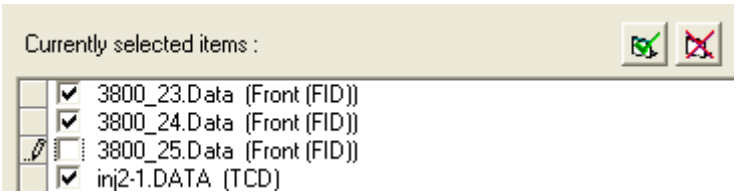
User can add chromatograms by selecting the Add chromatograms option, or all the chromatograms acquired within a sequence by selecting the Add chromatograms from a sequence, or all the chromatograms contained in a reprocessing list by selecting the Add chromatograms from a reprocessing list. The selected objects (chromatograms, sequences or reprocessing lists) are then listed in the Selected items field.



Then click on NEXT. The screen, listing the chromatograms to sign is displayed:

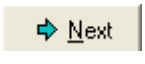


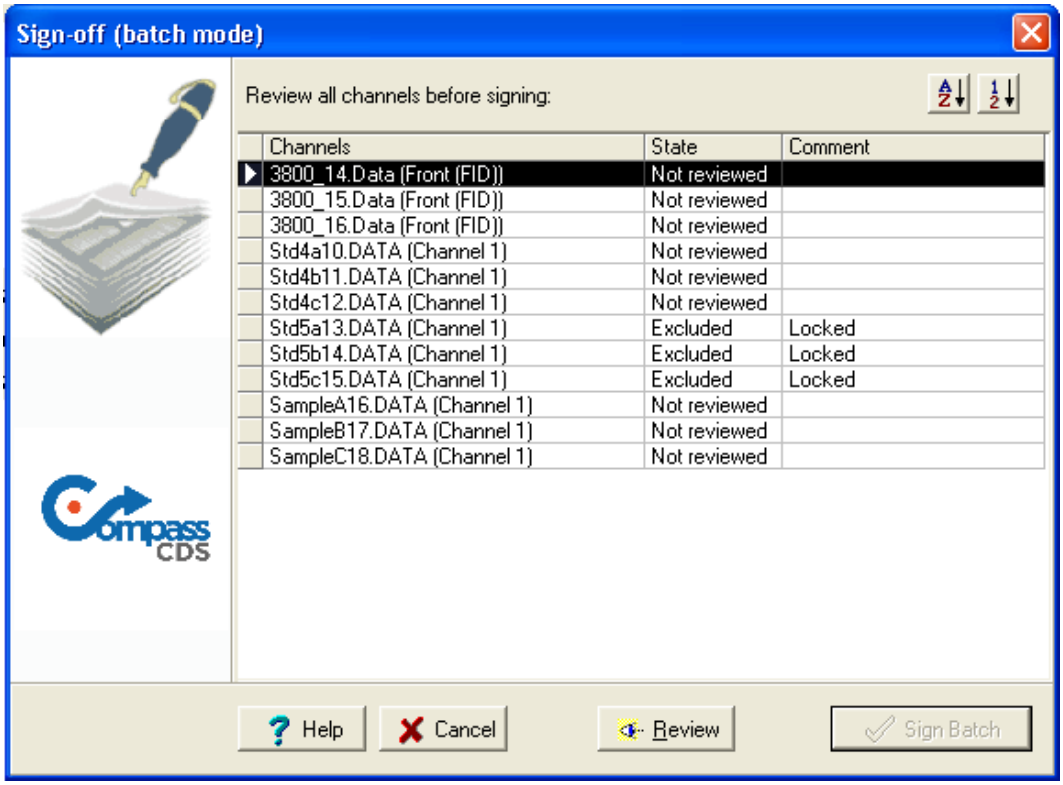
The chromatograms corresponding to the previous selection are listed in this screen; one line is added by channel. The user can remove some chromatograms from the list by unchecking the associated box. To check or uncheck several chromatograms in a single action, you can use the Shift and Ctrl keys, or extend the selection of the lines:



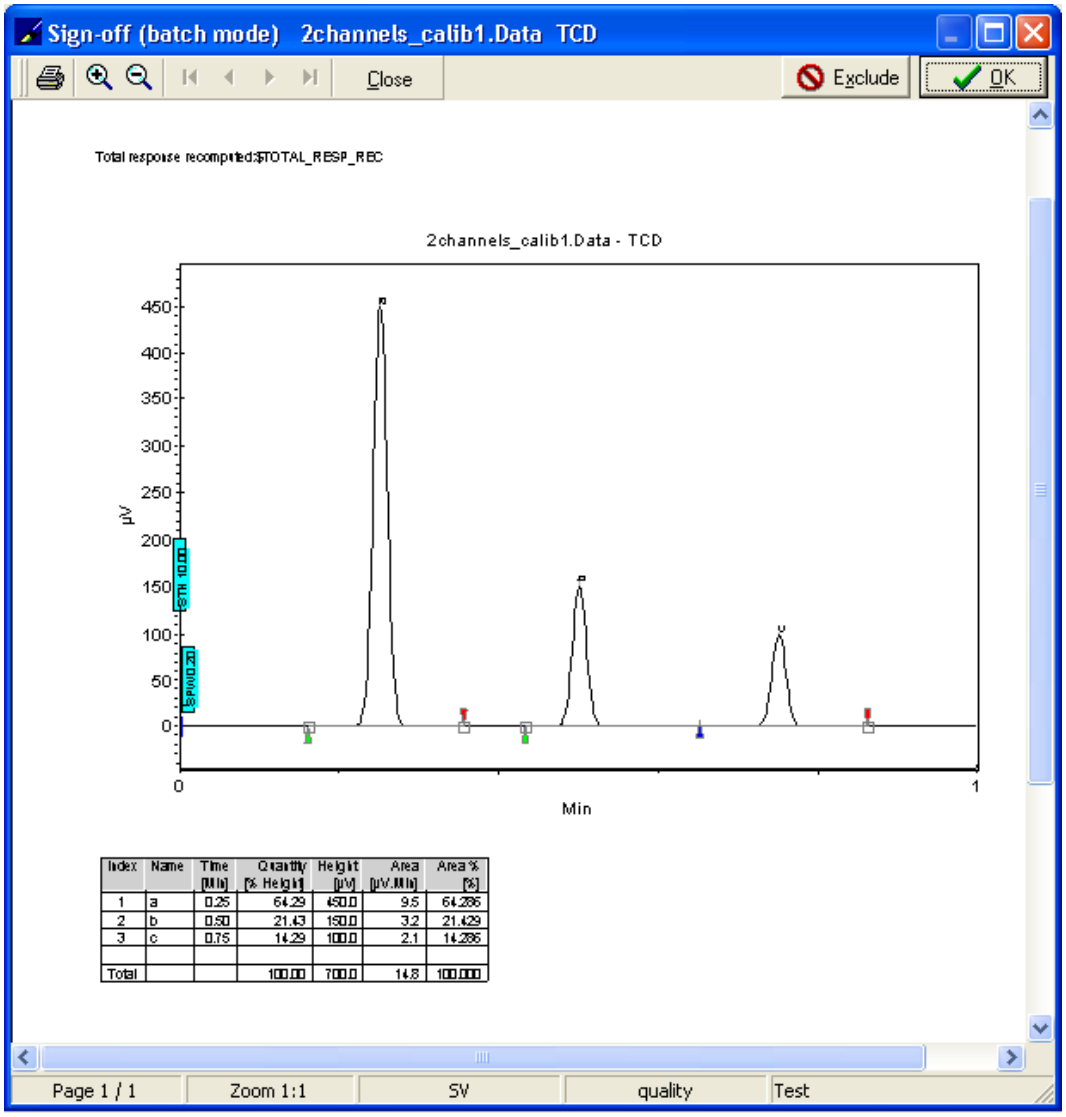
Then click on the Check selection icon or Uncheck selection icon .

It is also possible to sort the chromatograms either by name ( ) or by channel ( ), to make the selection easier.

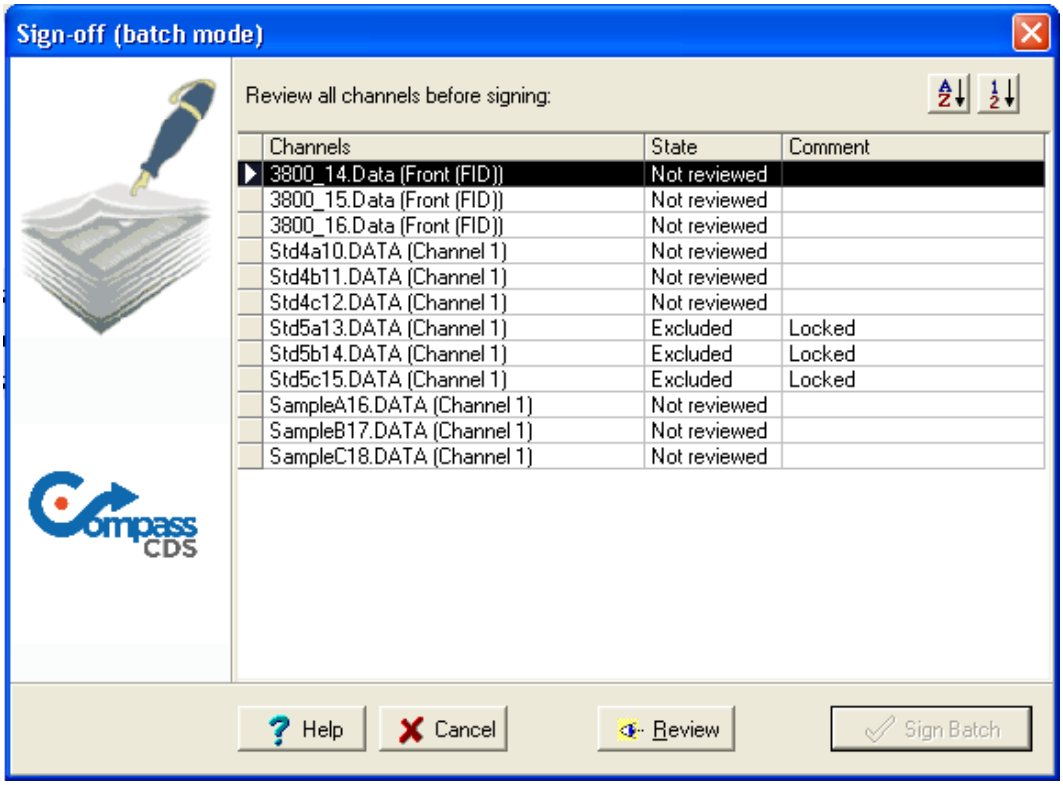
Once the chromatograms to sign have been selected, click on the  button. The following screen is displayed:



Click on the button to display the report of the first listed chromatogram.



Click on OK to accept to sign this chromatogram or on Exclude to exclude it from the batch of chromatograms to sign. Then the previous screen is displayed to show the signature progression:

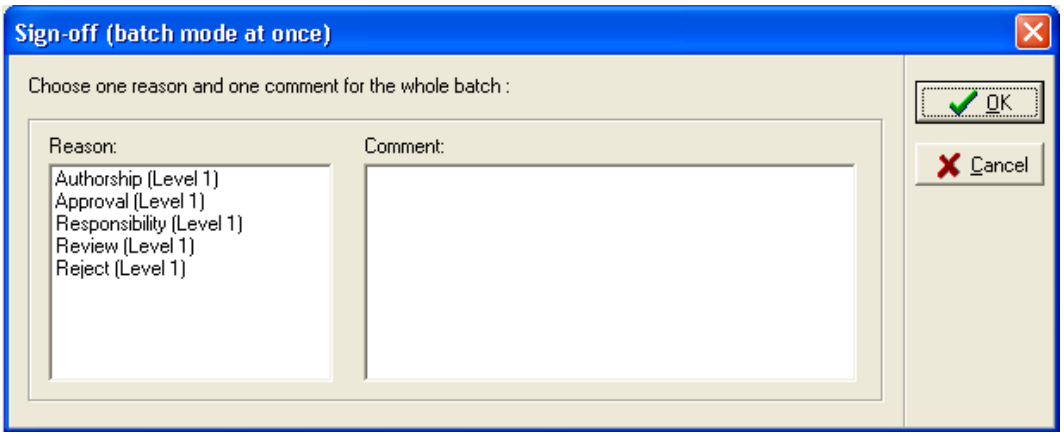


In case the user has 'Excluded' the chromatogram, 'rejected by user' is listed in the Comment column.

User has to select the

button until he has accepted or excluded all the listed chromatograms. Then the

button becomes available. By clicking on it, the following screen is displayed:

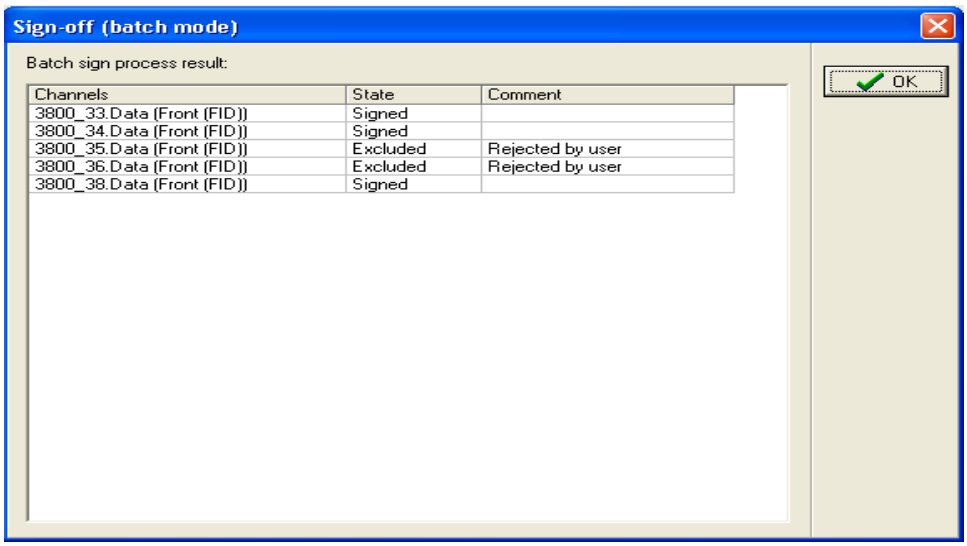


In this screen, the user selects the signature reasons wanted to assign to all chromatograms and optionally comments. Click on OK to perform the signature.

The user must enter the User Id and password in the corresponding fields, click on Validate to confirm the signature, then click on the Close button to exit this screen.

NOTE: Some users can sign as representative of a user, as in the single chromatogram process (see p 62). In that case, all the representative users must sign together.

The following screen is displayed to indicate whose chromatograms have been signed in the list.

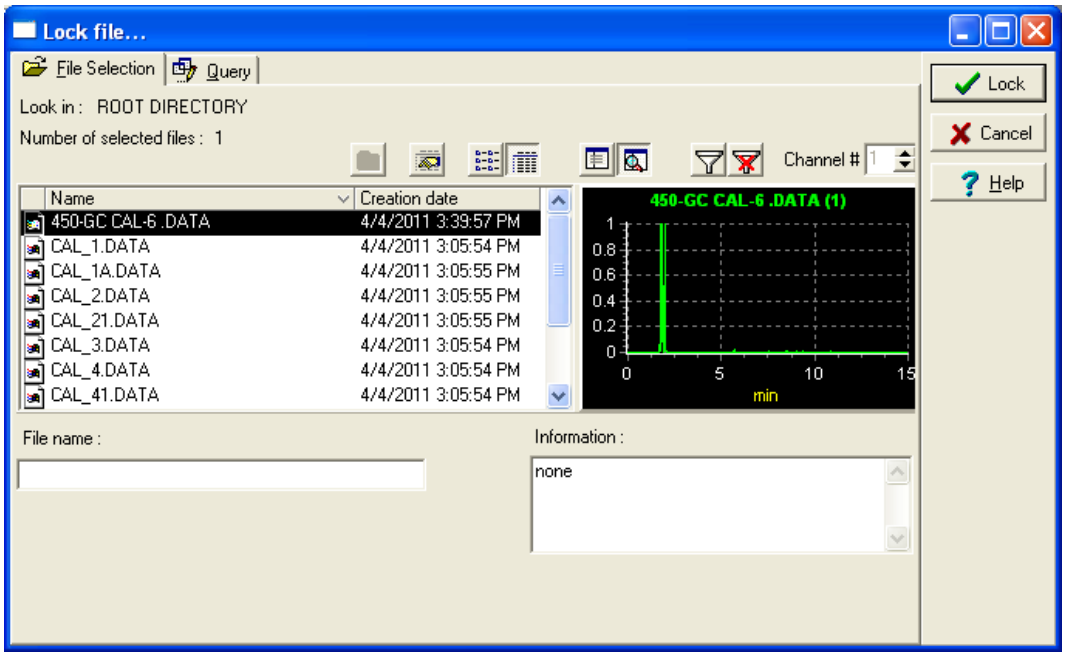


Lock/Unlock Chromatograms

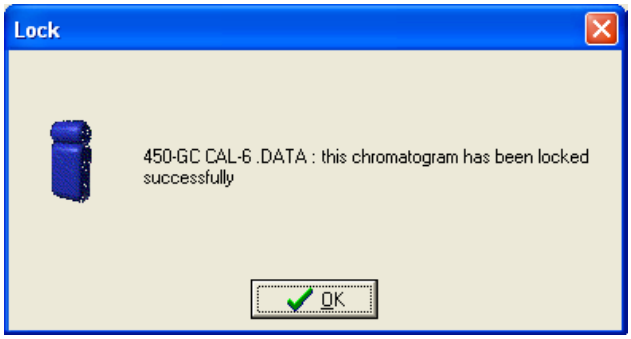
CompassCDS offers the possibility to lock (and then unlock) the chromatograms. A locked chromatogram can be open, printed, exported. A locked chromatogram can be modified but the modifications cannot be saved.

To lock one or several chromatograms, click on the icon or choose the FILE/LOCK CHROMATOGRAM menu.

The following screen appears:

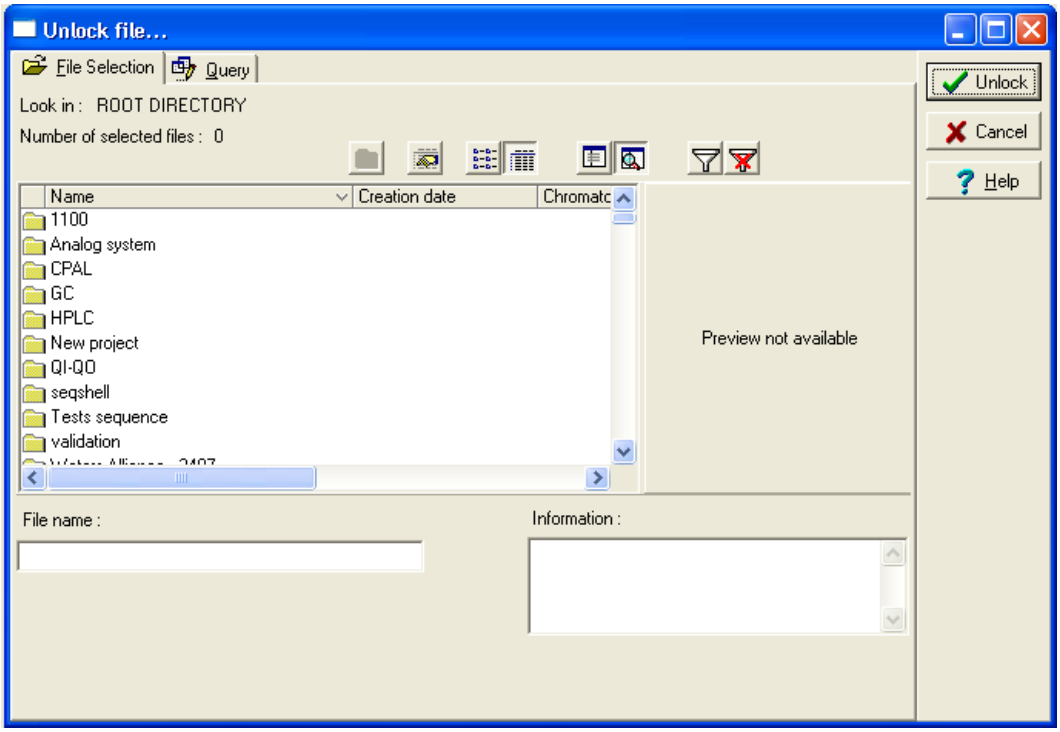


Choose the chromatograms to lock and click on the Lock button. A confirmation message appears as soon as the chromatograms are locked.

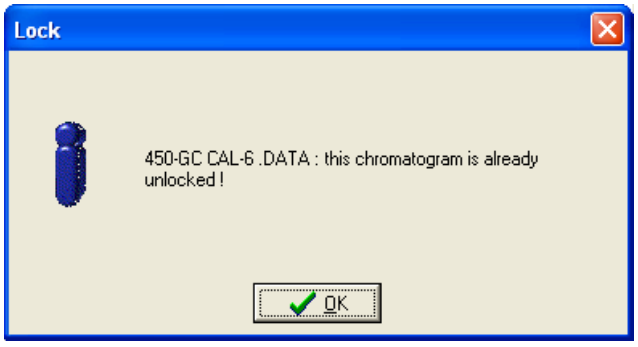


To unlock one or several chromatograms, click on the icon or choose the FILE/UNLOCK CHROMATOGRAM menu.

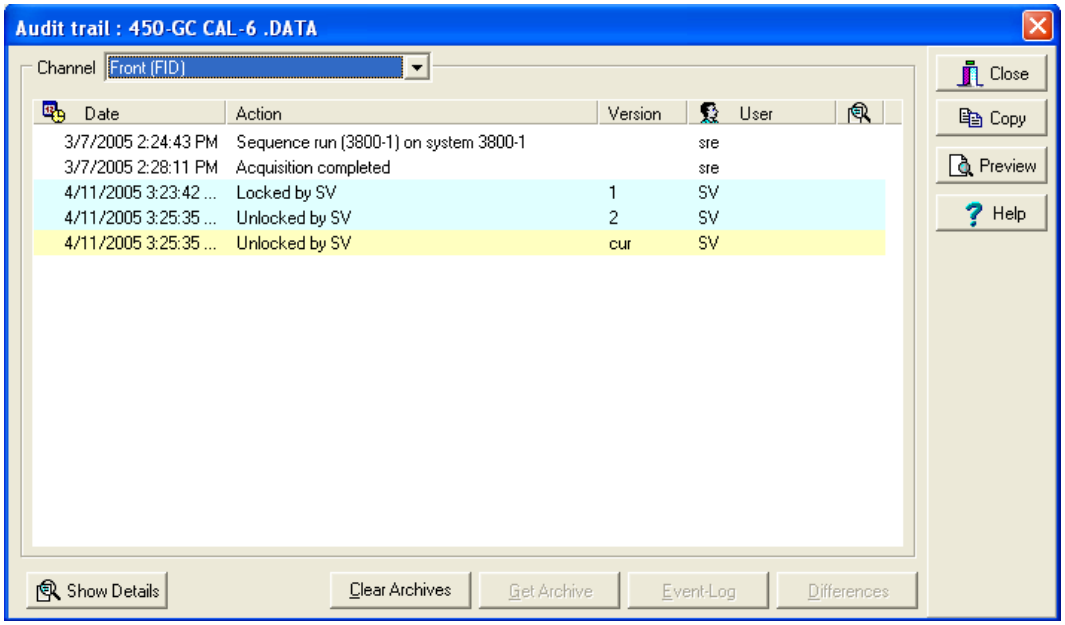
The following screen appears:



Choose the chromatograms to unlock and click on the Unlock button. A confirmation message appears as soon as the chromatograms are unlocked.



In the chromatogram audit trail, the lock and the unlock actions are listed as displayed in the following screen:


Audit trail : 450-GC CAL-6 .DATA
Channel
Front (FID)
Date
Action
Version
User
3/7/2005 2:24:43 PM
Sequence run (3800-1) on system 3800-1
sre
3/7/2005 2:28:11 PM
Acquisition completed
sre
4/11/2005 3:23:42 ...
Locked by SV
1
SV
4/11/2005 3:25:35 ...
Unlocked by SV
2
SV
4/11/2005 3:25:35 ...
Unlocked by SV
cur
SV
Close
Copy
Preview
Help
Show Details
Clear Archives
Get Archive
Event-Log
Differences

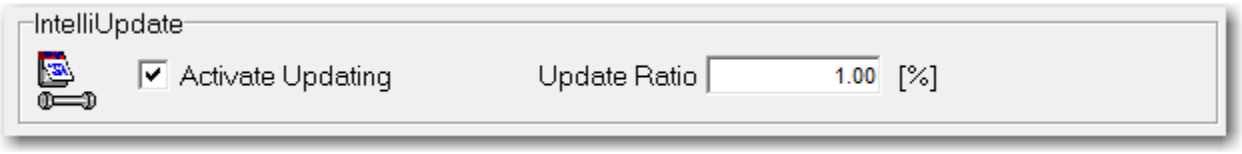
Advanced Parameters

This section concerns very particular applications used to answer specific user needs, and are not defined by default, during the software installation.

IntelliUpdate

CompassCDS contains an option enabling the user to simulate the ageing of a chromatographic column, by modifying automatically the theoretical peak and group retention times, as well as the integration event times in the method after an acquisition.

To activate this option, the user must be assigned a profile (CompassCDS Configuration Manager) containing the IntelliUpdate option in the Method directory.



An added part, named IntelliUpdate appears in the acquisition part

The user checks the ‘Activate column Ageing’ box to activate the function, and enters in the Ratio box the shift percentage to apply during the new retention time calculation of peaks and groups and integration event times (details of the calculation are described in this section).

‘IntelliUpdate” is applied from one acquisition to another, that means that at the end of an acquisition with this option, the method is automatically modified, and new parameters will be used for the next acquisition with this method.

IntelliUpdate is applied only during acquisitions (Quick Start and sequence). If a chromatogram is reprocessed via the ‘Integrate’ (F5), ‘Reprocess’ (F6) function or via a reprocessing list, no change in the peak and group identification and in the integration event tables is made in this method.

Once the chromatogram has been acquired, the ‘IntelliUpdate” part of its method is no longer accessible, so it cannot be modified.

To apply calculation of ‘IntelliUpdate” the user is required to define reference peaks in the peak identification table. If no reference peak is defined, or if at least one of the reference peaks defined is not found in the chromatogram, the ‘IntelliUpdate calculations will not be done.

Calculation details:

For all the peaks defined in the identification table and present in the chromatogram, the time limit of groups and the integration events time, the following calculation is applied:

$$RT'_{ID} = K\% \times RT + (1 - K\%) \times RT_{ID}$$

Where:

Identified peaks:

RT'_{ID}	represents the theoretical peak retention time calculated according to the ‘IntelliUpdate” function, and displayed in the peak identification table of the updated method (after acquisition).

RT	represents the real retention time of the present peak, displayed in the result table, or the interpolated retention time of missing peak according to the reference peak shift (see above equation).
K%	represents the update percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the theoretical retention time of the peak defined in the peak identification table of the acquisition method.

Integration events:

RT'_{ID}	represents the time of the integration events calculated according to IntelliUpdate function, displayed in the integration part of the updated method (after acquisition).
RT	represents the integration event times interpolated according to the reference peak shift (see above equation).
K%	represents the update percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the integration event times defined in the integration part of the acquisition method.

Groups:

RT'_{ID}	represents the calculated group time limits according to column ageing function, displayed in the group identification table of the updated method (after acquisition).
RT	represents the interpolated limit time of groups according to the reference peak shift (see above equation).
K%	represents the ageing percentage. It is the ratio value entered in the acquisition part of the method.
RT_{ID}	represents the theoretical time limits of groups defined in the group identification table of the acquisition method.

The RT time used for the integration events time, group time limits and retention time of the peak defined in the identification table, but missing from the chromatogram is interpolated according to the reference peak shift. Here is the used equation:

$$RT = RT_1 + (RT_{ID} - RT_{ID1}) \times \frac{RT_2 - RT_1}{RT_{ID2} - RT_{ID1}}$$

where:

RT	Is the time used in the IntelliUpdate formula.
RT1	Is the retention time of the previous reference peak.

RT2	Is the retention time of the next reference peak.
RTID	Is the theoretical retention time of non-reference peaks (defined in the identification table), or the integration event time, or the time limits of groups.
RTID1	Is the theoretical retention time of the previous reference peak, defined in the identification table?
RTID2	Is the theoretical retention time of the next reference peak, defined in the identification table?

NOTE: If peaks are eluted before the first reference peak, RT1=RTID1= 0 and the index 2 is attributed to the next reference peak.

$$RT = RT2 \times \frac{RT_{ID}}{RT_{ID2}}$$

If a peak is eluted after the last reference peak, RT1 and RT2 represent the retention time of two reference peaks eluted before the peak of interest.

A file is automatically generated after the first acquisition is made with a method using 'IntelliUpdate' function, in which the changes of times (peak RT, group time limits and integration event times) are listed. This file is updated after each acquisition is made with the same method. It is generated in the project directory containing the method, and is named the same as the method it comes from with the METH_CA extension. This file is readable as a text file (Notepad).

Remote Sequence

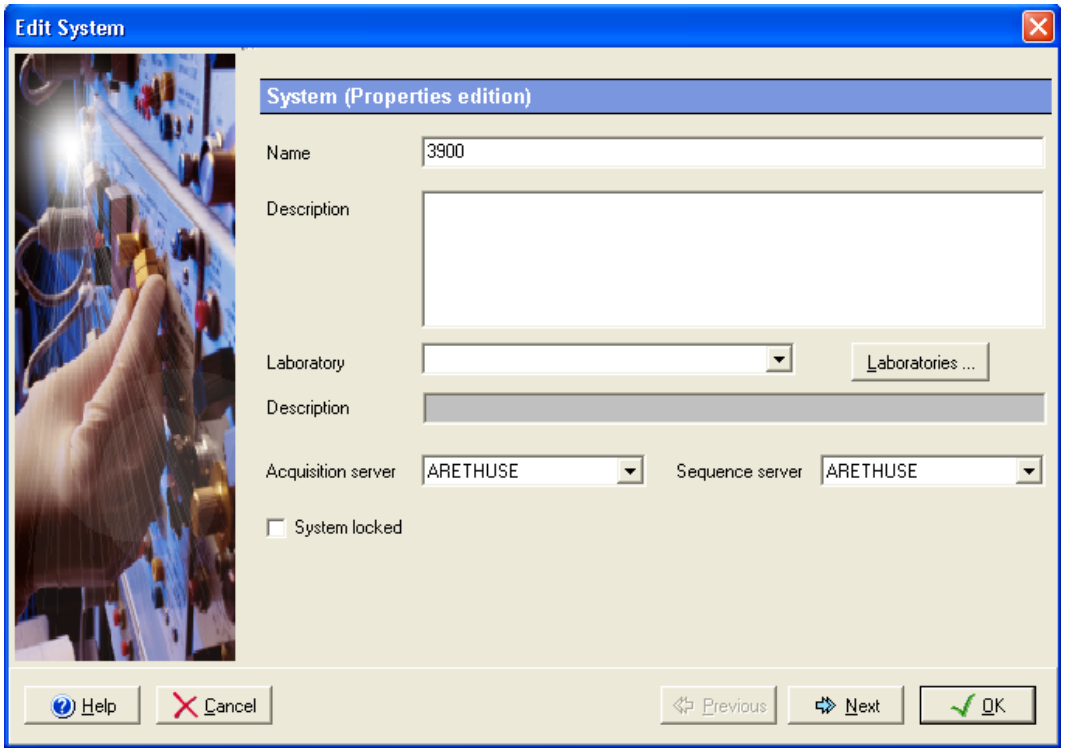
The aim of the 'Remote SequenceRemote Sequence' is to start a sequence on any workstation declared in the domain of work (in the CompassCDS Configuration Manager), and to close the CompassCDS session on this workstation while the sequence is running. It is also possible to disconnect from Windows session without stopping the Remote Sequence.

Configuration

The 'Remote SequenceRemote Sequence' runs as a service of the chromatographic system. One service is created for each system and is named "Remote SequenceRemote Sequence Engine-Systemname" (Systemname represents the name of the system). The services are accessible from the CONTROL PANEL /ADMINISTRATOR TOOLS / SERVICES menu.

At each start of an Remote Sequence, the corresponding service is automatically started on the sequence server, and is automatically stopped at the end of the sequence.

The sequence server is declared in the CompassCDS Configuration Manager in the system object:



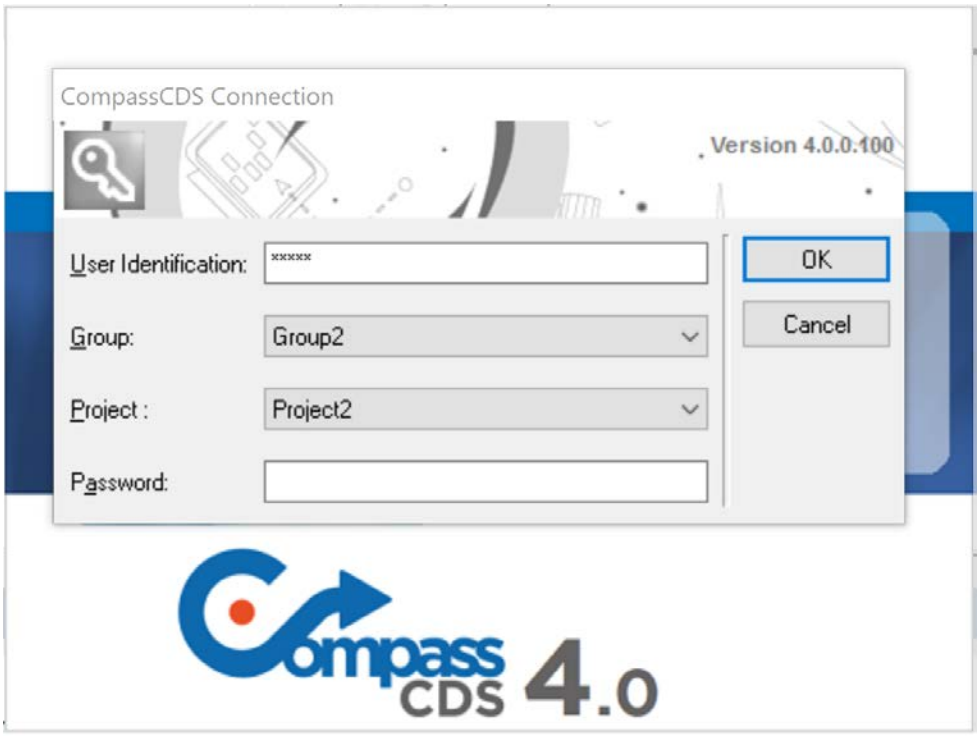
How to Use the Remote Sequence

Connection and Main Screen

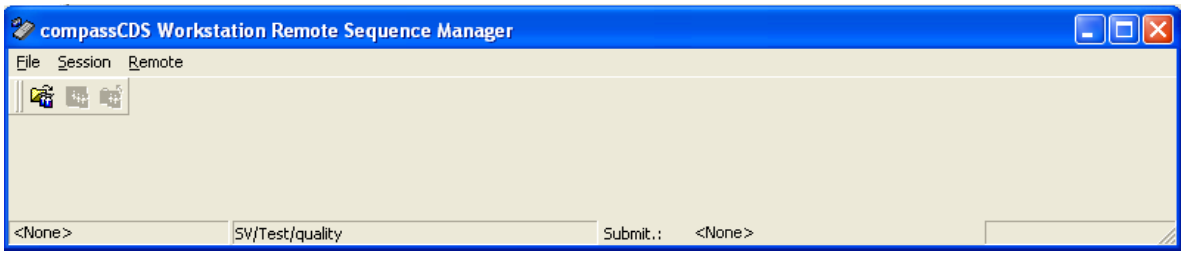
The Remote Sequence software may be opened from CompassCDS Acquisition Menu.

NOTE: The User must have a profile allowing him to start the Remote Sequence Manager (in CompassCDS Configuration Manager: user profile: Sequence / Use remote sequence).

First the logon box is displayed:

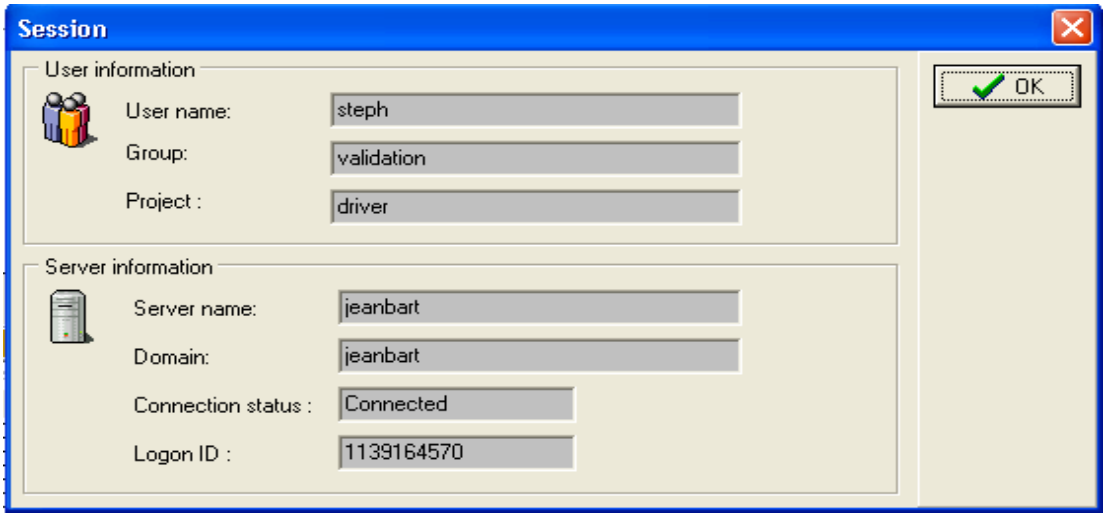


After entering a user name, the user can choose the project/group on which he wants to work and validate. The main screen is displayed:



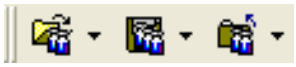
This screen contains three menus:

- **File menu:** allows the user to create, open, save, close a sequence, or quit the Remote Sequence.
- **Session menu:** allows the user to change the Session (New login) or to view properties:



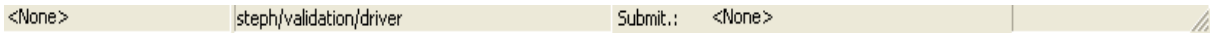
- **Remote menu**: allows access to the Queue status option, which lists all the acquisitions completed and their state. This also allows access to 'System log' option, listing the errors that may have occurred during the acquisition, or mentioning a communication problem with the chromatographic system or other problem.

A Toolbar:



Open sequence, save sequence, close sequence.

A task bar:



Sequence name user/group/project Sequence name by User State

The sequence name content is displayed on a green background, if the sequence displayed has been saved or in red if the changes were not saved.

The second case indicates the logon user/group/project.

The submit case indicates that the current sequence was initiated by 'user'. It has a green background if the current logon is the logon of the user who initiated it, and is red if it was initiated by another user. Note that if several Remote Sequences are opened with the first logon, only the first Remote Sequence opened, has a green background.

The state case shows the sequence state: starting, stopping.

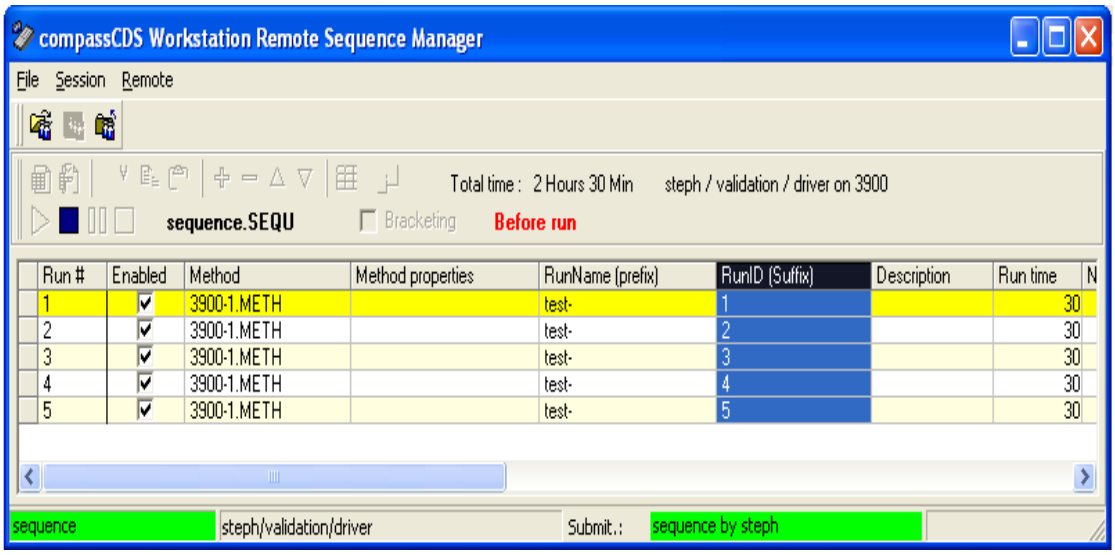
Running a Sequence

The sequence is the same as the sequence in CompassCDS: same grid, same functions. The user should consult the corresponding chapter in the manual (page 145).

External sequence: rules of work

- When a user starts a sequence, he becomes the 'Owner' of this sequence. That gives him all the rights (modify, pause, stop and reset the sequence). Note that changes are only possible when activating the pause button, otherwise the save function is not accessible.

The sequence is displayed as shown in the following picture:


compassCDS Workstation Remote Sequence Manager
File Session Remote
Total time : 2 Hours 30 Min
steph / validation / driver on 3900
sequence.SEQU
Bracketing
Before run
Run # Enabled Method Method properties RunName (prefix) RunID (Suffix) Description Run time N
1 3900-1.METH test- 1 30
2 3900-1.METH test- 2 30
3 3900-1.METH test- 3 30
4 3900-1.METH test- 4 30
5 3900-1.METH test- 5 30
sequence
steph/validation/driver
Submit.:
sequence by steph

The submit field of the task bar is displayed on a green background to remind the user that he started the sequence and that he is its owner.

- If another user connects on another workstation and opens the same sequence, he will only have viewing rights. The submit field of the task bar will have a red background, indicating that this user is not the owner of the sequence and that he has no rights. The stop, pause, reset & start buttons are not accessible to this user. If he makes some changes in the sequence (adds lines for example), these changes will not be taken into account since he is not the owner of the sequence.

Nevertheless 'Non-Owner user' can have rights to change and to save the sequence, if the original owner closes the sequence. However, the non-owner cannot stop the sequence, restart or reset it.

Note that if a non-owner user of a sequence has the 'Stop any running acquisition' profile (declared in the CompassCDS Configuration Manager), he has the full rights (stop, start, save, reset) once the owner has closed the Remote Sequence screen.

Report Printing

The report printing is managed by the workstation on which the Remote Sequence is started. This means that the default printer defined for the Windows user (connected to workstation) will be used for printing, in the sequence. If another user connects to this workstation and the printer associated to his Windows profile is different, reports will be printed on his printer (even if he has not opened the Remote Sequence).

The Windows profile of the user connected to the workstation defines the printer.

To print reports, the workstation must always be connected under a Windows session. If no user is connected on a Windows session, acquisitions will be performed, but no printing will be done.

NOTE: To change Windows log-on, select the "Close all programs and log on as a different user." This is the option in the start menu to avoid stopping the computer.

Retention Index

CompassCDS has an option enabling retention indices calculation. Retention index is defined by reference to two standards of homologous series, whose peaks bracket the compound of interest. Calculation is based on Kovats principle (for alkanes with isothermal temperature) extended to other chemical series (alkenes, esters…) and temperature programs.

Reference compounds can be either analyzed simultaneously to unknown compounds, or separately, provided, that analytical conditions remain identical.

This option allows identification not only with retention time, but also with retention indices.

Configuration

To activate this option, the user must be assigned a CompassCDS Configuration Manager user profile. Check the "Edit peak identification parameters" and "Retention index" options in the "Method" subdirectory of the user profile.

Two options are then available in the "Peak identification" part of the method: "Retention index" and "Identification using index".

Check the "Retention index" box to use the retention index option.

- A column appears in the identification table: Ret. Index. It allows the user to enter retention indices in the peak identification table.
- A new menu RETENTION INDEX appears in the main toolbar.
- The option "Identification using indices" becomes active. If it is checked, two additional columns appear in the identification table: Abs window (ret.ind), Window % (ret.ind). Abs window (min) and Window % columns disappear.

Reference Table Building

To calculate retention indices in an unknown chromatogram, a "Reference table" must be created. In a homologous series of chemical compounds, this table links retention time to retention index.

A reference table consists of two parts:

- Analytical conditions of chromatogram acquisition.
- Reference identification table, which lists the entire homologous series information (retention time, retention index, identification window, etc.).

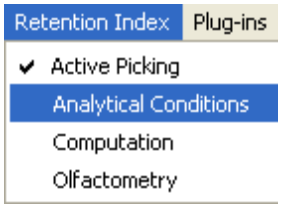
Reference Analytical Conditions

Retention index calculation can only be done between chromatograms whose analytical conditions are identical. So, reference analytical conditions must be created.

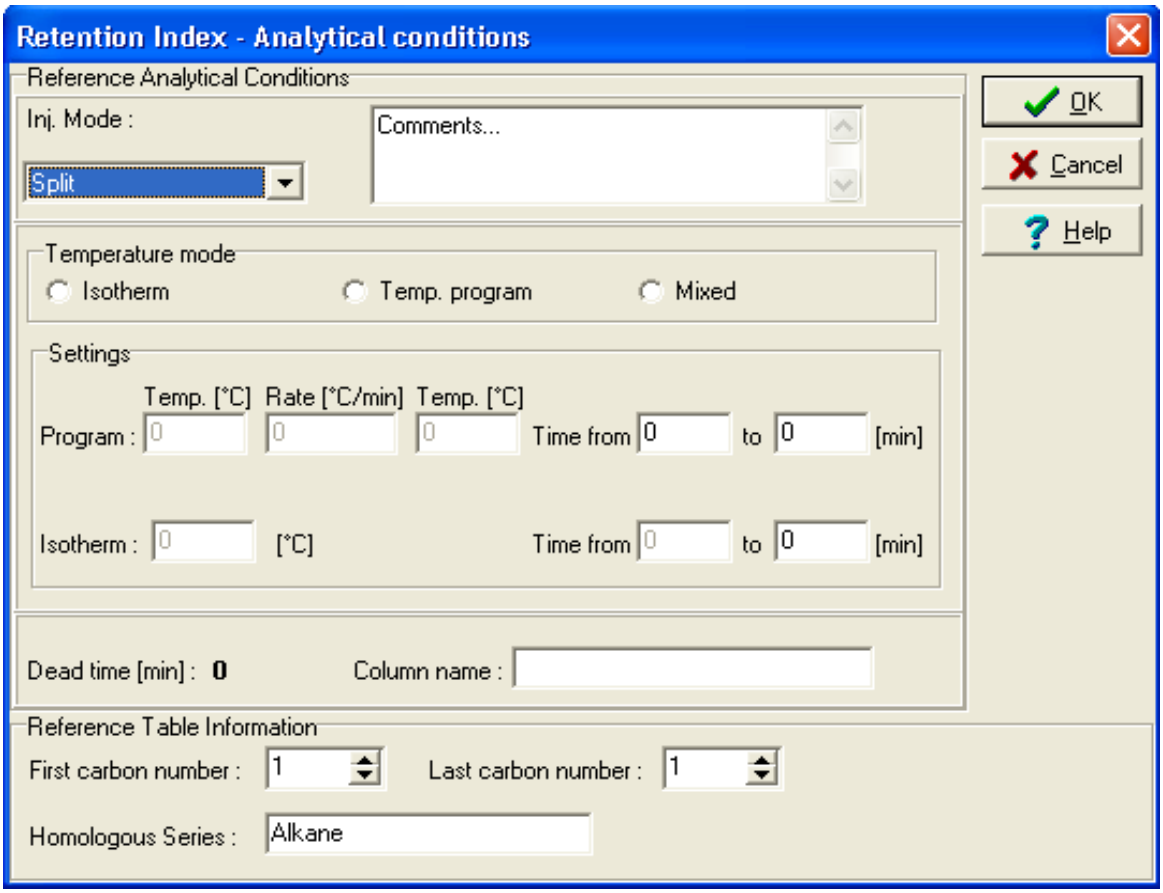
Open a method.

In the peak identification table, check "Retention index" option and possibly the "Identification using index" one.

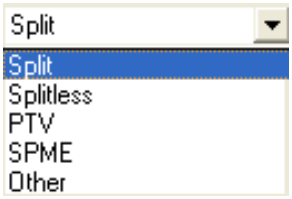
Select the RETENTION INDEX / ANALYTICAL CONDITIONS menu.



The following screen appears:



Inj mode: select the injection mode among: Split, Splitless, PTV, SPME or Others



Comments: Enter comments if necessary

Temperature mode: select temperature conditions of the acquisition. Three temperature modes are available:

- **Isotherm:** enter the temperature.
- **Temp. Program:** enter initial and final temperatures and the rate. Only one rate is allowed.
- **Mixed:** a rate can only be followed by an isothermal level. Enter temperature, rate, and initial and final program time.

Dead time: The column dead time is imported from the acquisition part of the method, it is impossible to enter this data manually.

Column name: enter column name.

Reference table information: to specify reference compounds.

- **First carbon:** carbon number of the first reference compound.
- **Last carbon:** carbon number of the last reference compound.
- **Homologous series:** name of homologous series.

NOTES: If the last carbon number is less than the first, it appears on a red background to inform user of the inconsistency.

Each compound within the defined range (from first carbon number to last carbon number) must be present, in order to construct the Reference Identification Table

Save the method when all fields have been filled out.

Reference Identification Table

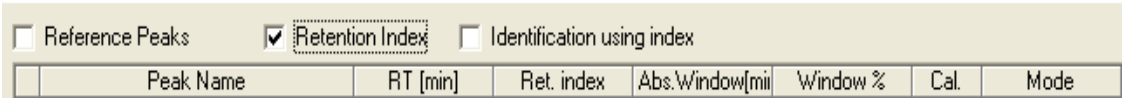
When reference analytical conditions have been defined in the method, reference chromatogram (chromatogram containing the peaks of interest of the homologous series) can be either reprocessed (F6) or acquired with this method.

Then reference peak identification table can be built.

Peaks can be identified according to their retention time or their retention index:

If the Retention index option is checked and identification using index is unchecked, peaks are identified according to their retention time.

The following identification table appears:



Peak name: compound name.

RT: theoretical retention time of the compound.

Ret. Index: theoretical retention index of the compound.

Abs window (min): absolute identification window in minutes (according to retention time).

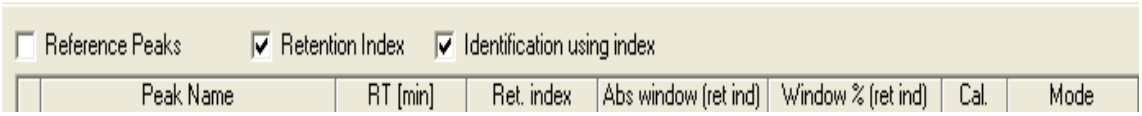
Window %: relative identification window in % (according to retention time).

Cal: check this box if the compound must be used for calibration.

Mode: identification mode.

If the Retention index AND Identification using index options are checked, peaks are identified according to their retention index.

The following identification table appears:



Peak name: compound name.

RT: theoretical retention time of the compound.

Ret. Index: theoretical retention index of the compound.

Abs window (ret ind): absolute identification window for retention indices.

Window % (ret ind): relative identification window in %, for retention indices.

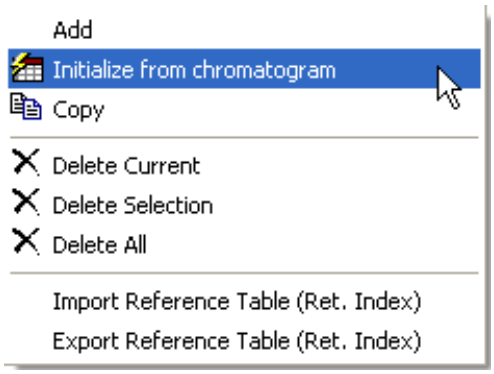
Cal: check this box if the compound must be used for calibration.

Mode: identification mode.

Once identification mode has been selected, identification table can be filled-in either with popup menu or peak picking:

- With identification table popup menu:

Initialize from chromatogram option fills in the identification table with chromatogram information.

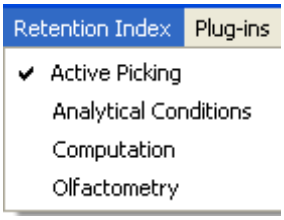


Peaks are automatically named and the retention index and filled according to what has been specified in the reference table information (name, first and last carbon).

Once peaks have been identified, the user must complete the other fields of the identification table.

- With peak picking from the chromatogram.

Active Picking option is accessible in the RETENTION INDEX / ACTIVE PICKING menu. It allows peak selection directly on the chromatogram.



Selected peaks are automatically named with homologous series names, and retention indices filled according to limits defined in the reference table information.

Peaks must be chronologically selected but if an error occurs, a chronological sorting is proposed.

Once peaks have been identified, the user must complete the other fields of the identification table.

NOTES: If data about peaks (name, retention time, retention index…) are known when the method is built, the identification table can be manually completed.

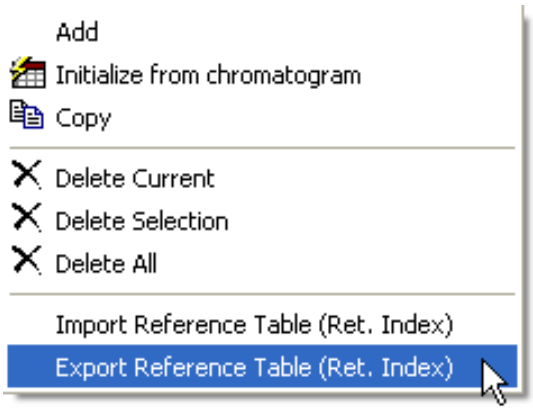
If a chromatogram is processed in retention index mode, and that it is subsequently reprocessed by a user who does not own the retention index profile, a sentence informs the inconsistency in the identification table.

Reference Table Export and Import

- Export:

Once reference analytical conditions and identification table have been built in a method, the reference table can be created in order to be used in other methods.

To export the reference table, select the popup menu Export reference table in the peak identification table of the reference chromatogram or method.

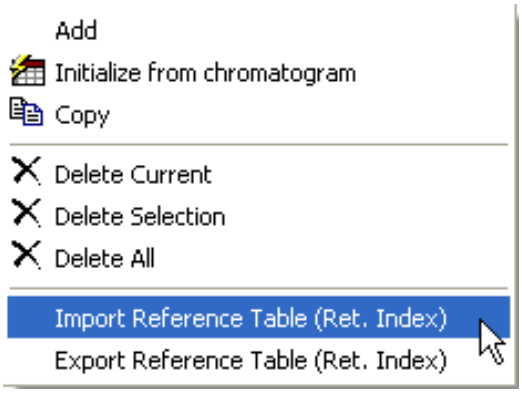


A file named ‘Chromatogram name.csv’ and readable in Excel is created, in the directory defined by the user during the export step. It contains the reference analytical conditions and the identification table.

- Import:

The reference table can be imported either in a method or in a chromatogram in order to process unknown chromatograms with retention indices.

To import the reference table, select the popup menu Import reference table of the peak identification table.



Retention Index Calculation

In the peak identification table, check "Retention index" box and if necessary "Identification using index" option.

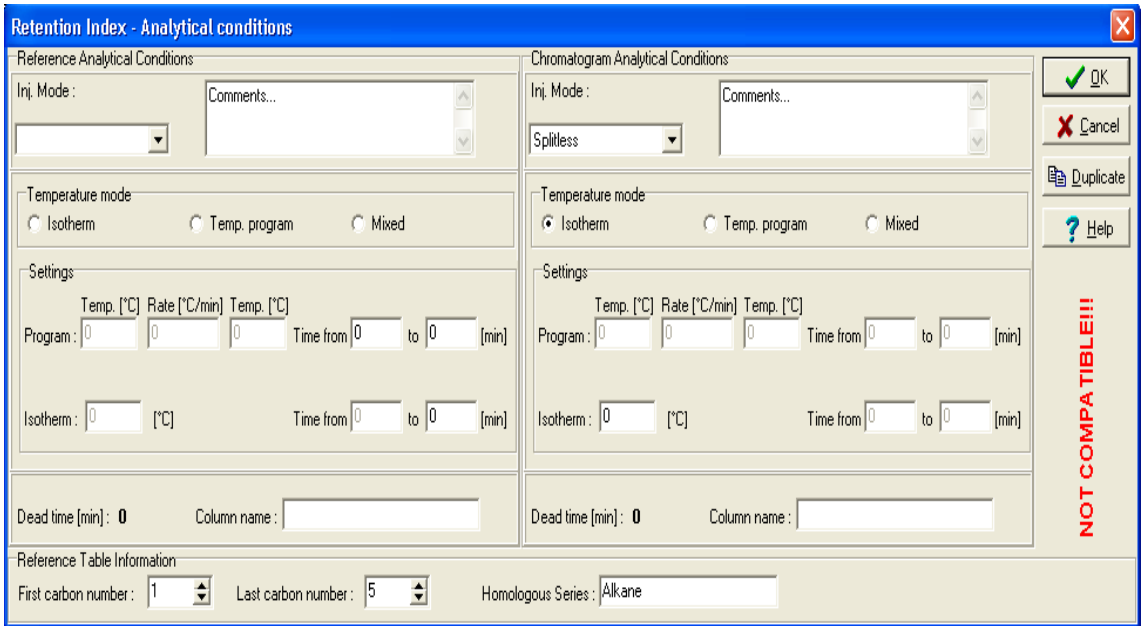
Processing Method

To calculate retention indices in a chromatogram, analytical conditions must remain identical.

Unknown chromatograms method must contain retention index reference parameters (table + analytical conditions). So, it is mandatory to either import a reference table via the popup menu "Import reference table" in the identification table, or to reprocess the chromatogram with a method which contains a reference table.

The identification table is then filled in with reference chromatogram peaks.

Select RETENTION INDEX / ANALYTICAL CONDITIONS menu, the following screen appears:



Reference analytical conditions: It contains the analytical conditions of the reference. This part cannot be modified in the chromatogram.

Chromatogram analytical conditions: It contains the analytical conditions of the unknown chromatogram.

Reference table information: It contains all information about homologous series of chemical compounds.

Index retention calculation is processed only if analytical conditions between reference and chromatogram are identical. A message COMPATIBLE or NOT COMPATIBLE!!! is displayed in order to advise the user if calculation can be done or not.

NOTE: If a chromatogram is acquired with a method containing retention index parameters (reference table, analytical conditions), the Chromatogram Analytical Conditions part is identical to the Reference Analytical Conditions. If reprocessing a chromatogram not acquired with retention index parameters with a method containing Retention Index parameters, the user has to complete the Chromatogram Analytical Conditions screen.

The

button copies reference analytical conditions into chromatogram ones.

As soon as COMPATIBLE is displayed, the user can process his chromatogram (or).

Calculation

The retention index calculation depends on analysis temperature program (Isotherm, Program, and Mixed)

- Isotherm: $$i_x = 100 * \frac{\log(t'_x) - \log(t'_n)}{\log(t'_{n+1}) - \log(t'_n)} + 100 * n$$
- Temp. Program: $$i_x = 100 * \frac{t_x - t_n}{t_{n+1} - t_n} + 100 * n$$

Where:

ix: retention index of the peak of interest,

t'_x: relative retention time of the peak of interest,

t'_n: relative retention time of the previous reference peak,

t'_{n+1}: relative retention time of the next reference peak,

t_x: retention time of the peak of interest in minutes,

t_n: retention time of the previous reference peak in minutes,

t_{n+1}: retention time of the next reference peak.

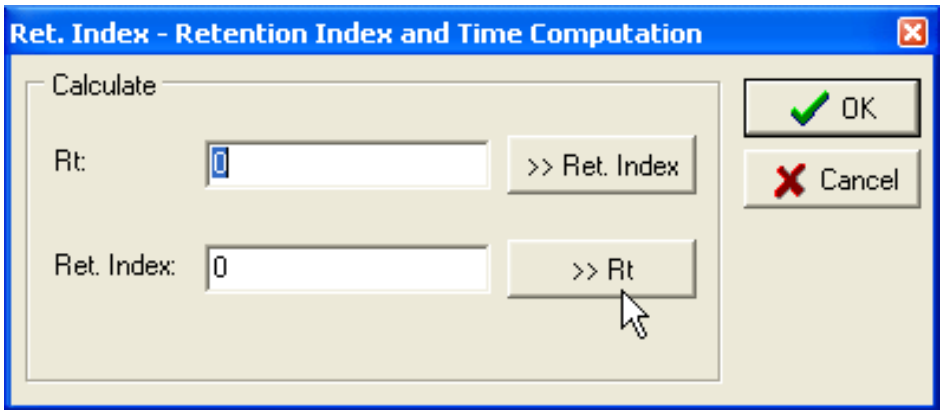
Where relative retention time (t') = retention time (t) - Dead time

- Mixed: In this program, a rate can only be followed by an isothermal level. During the rate, calculation is done with the temp. program formula. During the isothermal level, calculation is done with isotherm formula. If the peak of interest is bracketed with reference compounds

whose retention times are on different temperature programs, calculation is done with temp. program formula.

According to peak identification table information, the CompassCDS Chromatography Data System proposes an option which allows calculation of retention index from retention time, and the reverse calculation.

Select the RETENTION INDEX / COMPUTATION menu, the following screen appears:



If retention time is entered, select the

button, retention index will be calculated.

If retention index is entered, select the

button, retention time will be calculated.

NOTE: Calculations are allowed only in the retention time range or in the retention indices range defined in the identification table.

Variables

Two global variables are available:

Analysis Type [ANALYSISTYPE]: the type of analysis chromatogram or olfactogram.

Reference table name [REFTABLENAME]: the reference table name imported in the peak identification table.

Three peak variables are available to display calculation results.

RT Ind. [RETENTION_INDEX]: retention index of the compound.

Ret. Ind. offset [RETIND_OFFSET]: offset between theoretical and experimental retention indices.

Corr.Ret.Ind [RETIND_CORRECT]: corrected retention index according to reference compounds.

Results

Results are displayed in the Results-Peak report part of the chromatogram.

Select the "Report properties" popup menu to display Ret Ind., Ret Ind. Offset, Ret Ind. correct variables.

NOTE: If calculations have been processed within incompatible analytical conditions, the retention index column will appear in red.

On the chromatogram, compounds of the homologous series identified are named automatically.

CompassCDS Report Editor Report Style

Identification parameters are contained in the 'Method' object of the CompassCDS Report Editor Report style.

Results are contained in the 'Peak result' part of the CompassCDS Report Editor Report style.

CompassCDS ASCII Import

The CompassCDS ASCII Import allows converting ASCII data (.txt or .csv) into CompassCDS data files. This option is installed by default with CompassCDS; it is accessible via the FILE / IMPORT / ASCII FILES menu or the icon.

The details of this application are described in a separate user's guide, available in the CompassCDS / Manuals directory.

CompassCDS Print manager (PDF Export)

The CompassCDS Print Manager allows the user, when it is used as a post-processing, to combine printings and exports as PDF of the same chromatogram. Different printers, report styles and output paths can be chosen in the same configuration table. It also allows to export chromatograms as PDF and to choose the path where they are going to be stored on the computer.

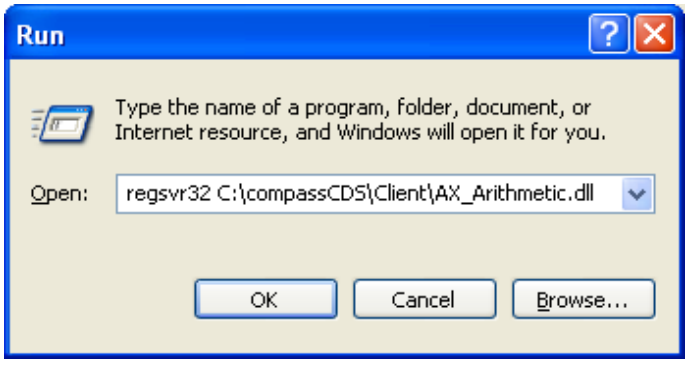
The details of this application are described in a separate user's guide, available in the CompassCDS / Manuals directory.

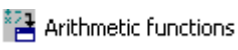
CompassCDS Arithmetic functions

The Arithmetic functions allow the user to realize operations (Addition, Multiplication, Subtraction, Division, and Weighted sum) between either chromatograms or chromatogram and real numbers.

The Arithmetic functions option is not installed by default with CompassCDS. The program is nevertheless available in the CompassCDS /Client directory.

To install it, select the START / RUN menu, enter 'regsvr32 ' then drag and drop the AX_Arithmetic.dll file from the COMPASSCDS / CLIENT directory:



To access the Arithmetic functions options, select the icon then the  sub-menu. The details of this application are described in the CompassCDS Arithmetic Functions Plug-in User Guide..

Procedures

This section gives actual examples of various procedures:

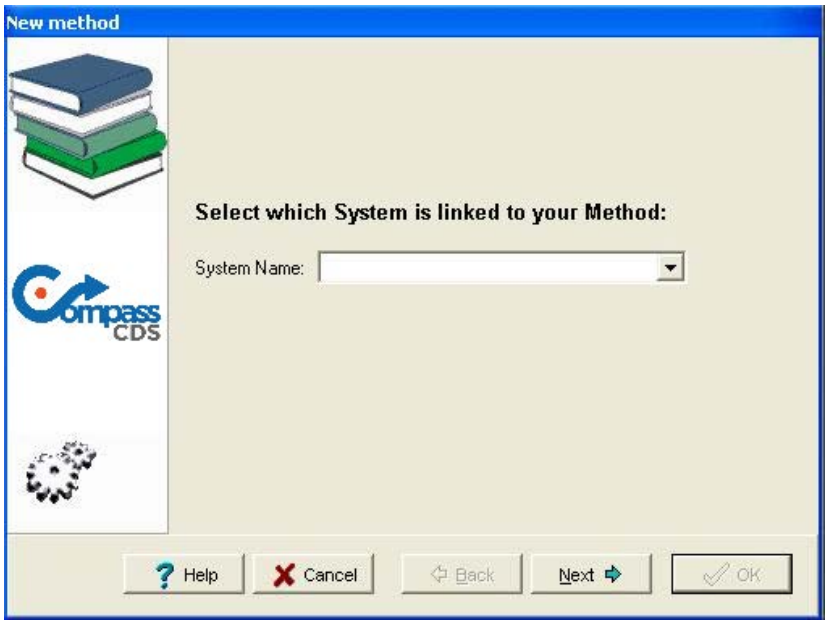
- How to acquire a chromatogram.
- How to program sequential analyses: the sequence.
- Creating a process method (integration, identification, quantification and printing).
- How to reprocess a chromatogram (integrate, quantify, print a report for a standard or an unknown sample).
- How to create a calibration curve.
- How to create a customized report.

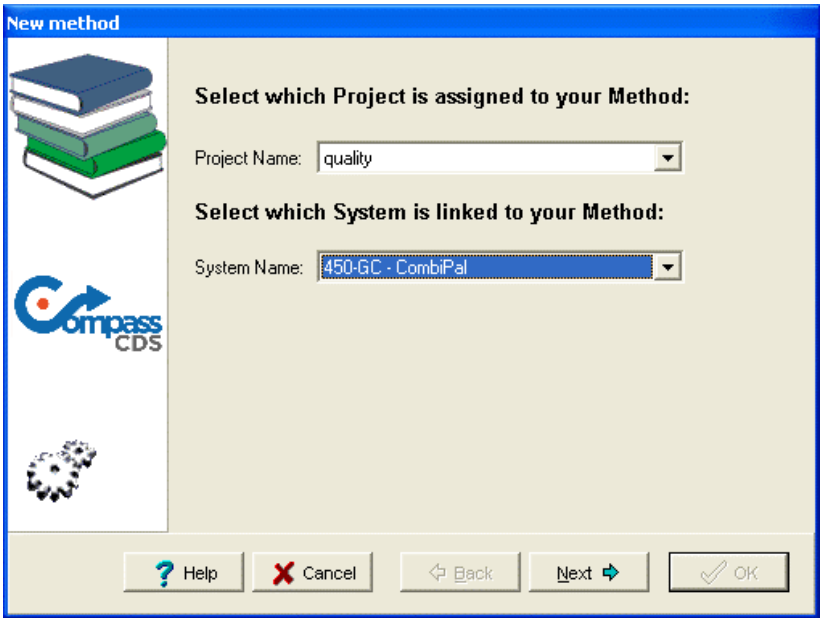
How to Acquire a Chromatogram

1. First create a method containing at least the control and acquisition parameters. Once the method has been created and saved, the acquisition can be started.

   Select FILE / NEW / NEW METHOD

   One of the following screens is displayed, depending on the way you log on to the CompassCDS Chromatography Data System, either in “all projects” or in a defined project.





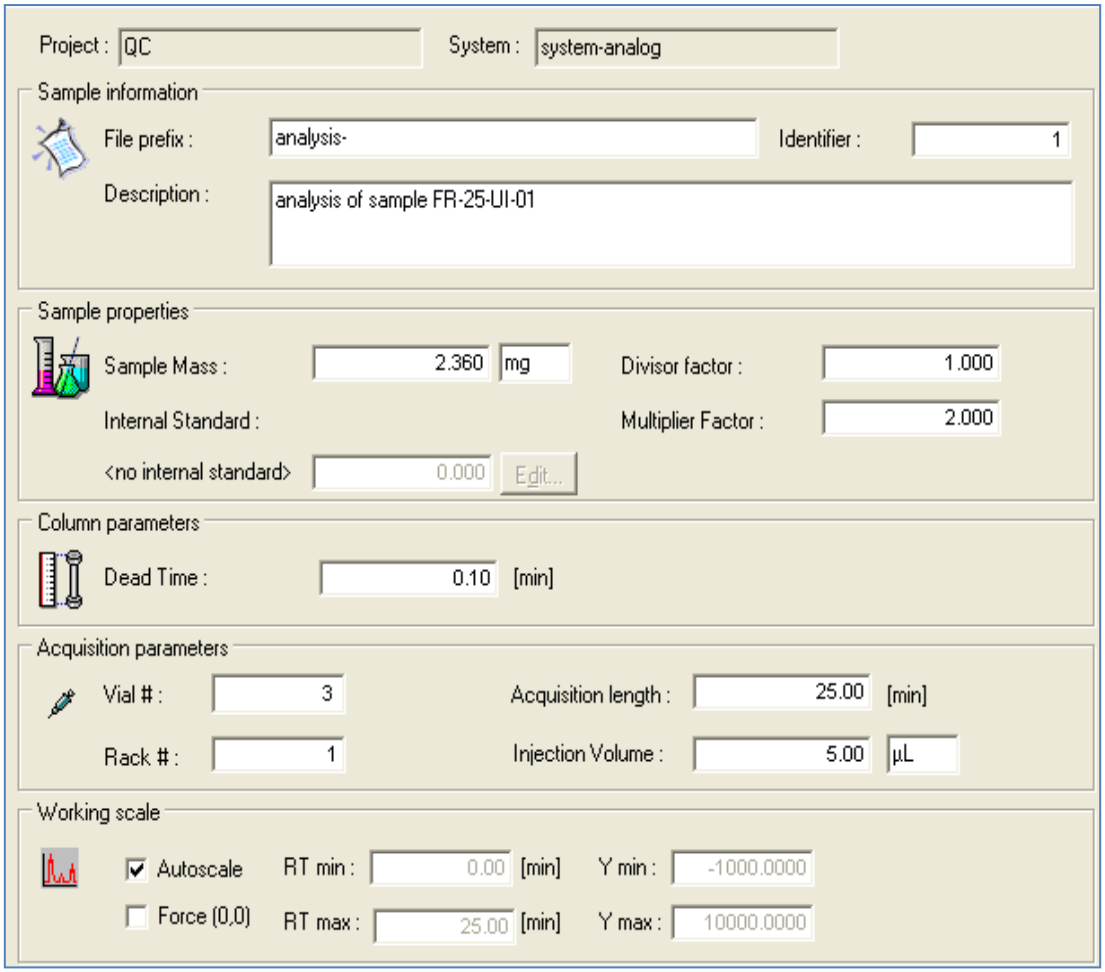
- Define either the name of the project linked with the method and the name of the system, or only the name of the system. The method is created and then displayed in the browser.
- Enter the control and acquisition parts of the method:

Control: This section depends on the chromatographic system and whether it is controlled or not by CompassCDS. Define:

The acquisition rate (number of points acquired per second).

- Start mode: “start on trigger” if the start signal is triggered by user (click on the chromatograph’s start button) or by an autosampler, or “start immediately” if CompassCDS triggers the start.
- The control parameters in the case of a controlled system.

  Acquisition:

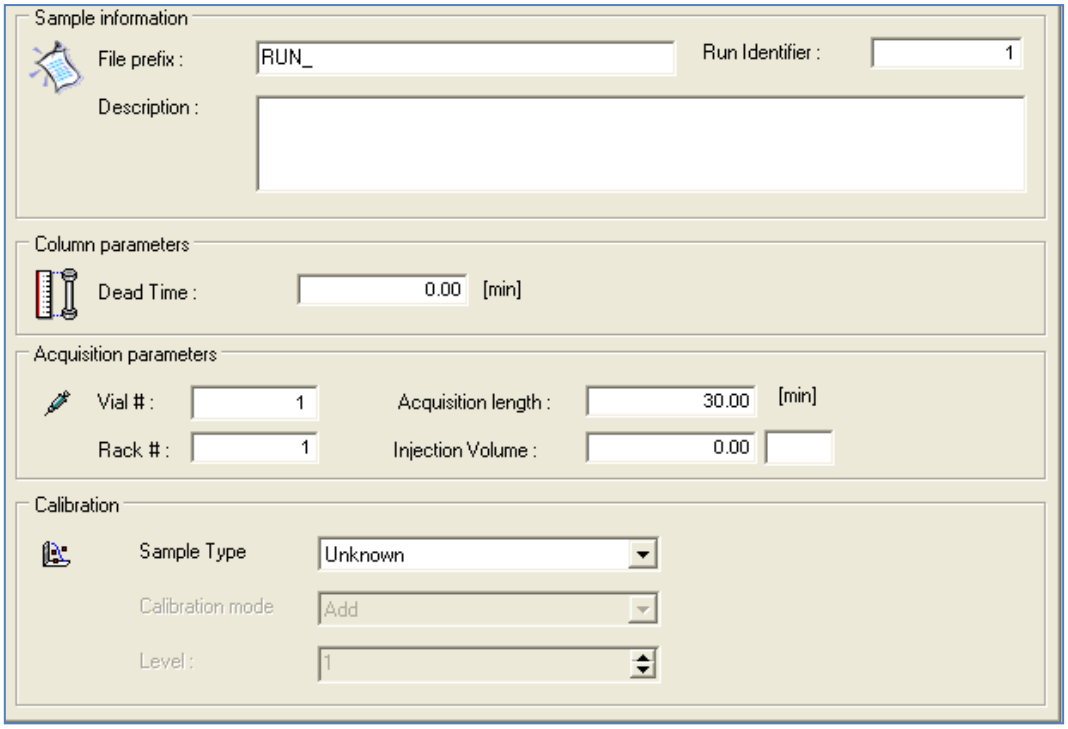


Complete at least the following fields: File prefix and Identifier, corresponding to the entire chromatogram name, and Acquisition length.

Save the method.

Start the acquisition (see page 139)

Press the button. The following screen is displayed:



If the system is using an autosampler controlled by the CompassCDS, define the injection volume, the vial position, the rack number (if required, otherwise leave at 0 as default), then click on the START button. If an Internal START is defined, CompassCDS controls the START; if an "external START" is defined (manual injection), inject and then press the START button on the chromatograph.

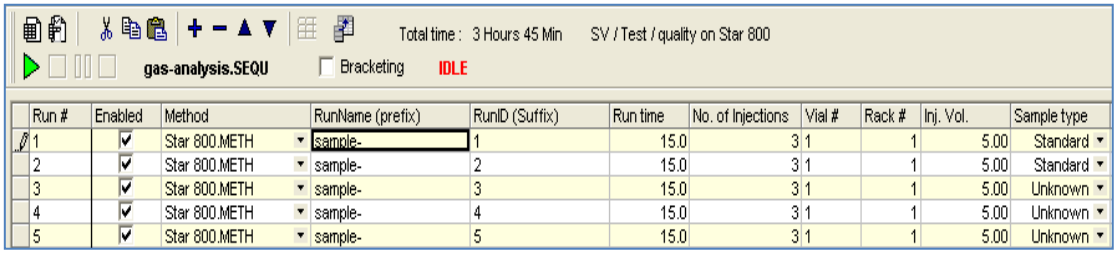
How to view the current acquisition:

In the "system" tab, select the system (click with the mouse on the left of the system name).

How to Define a Sequence for Analysis Execution

1. Define an analysis method. A minimal method is enough for an acquisition (page 241), but it is also possible to process automatically (identification, quantification, report printing, etc.) by using a more elaborate method.

   Create a sequence: menu FILE / NEW / NEW SEQUENCE, complete the displayed creation wizards (page 145), by entering the used system name, the number of lines (corresponding to the number of samples) and the sequence name. The sequence is displayed.
   Complete the sequence (page 147).



Run #	Enabled	Method	RunName (prefix)	RunID (Suffix)	Run time	No. of Injections	Vial #	Rack #	Inj. Vol.	Sample type
1	☑	Star 800.METH	sample-	1	15.0	3	1	1	5.00	Standard
2	☑	Star 800.METH	sample-	2	15.0	3	1	1	5.00	Standard
3	☑	Star 800.METH	sample-	3	15.0	3	1	1	5.00	Unknown
4	☑	Star 800.METH	sample-	4	15.0	3	1	1	5.00	Unknown
5	☑	Star 800.METH	sample-	5	15.0	3	1	1	5.00	Unknown

Some fields must be completed before starting the sequence:

The method name,

The RUN NAME,

The RUN ID,

The RUN TIME.

All this information is automatically imported from the method acquisition part if defined.

Specify in the ‘sample type’ column whether the chromatogram is a ‘blank to be subtracted’, a ‘standard’ (for automatic creation of calibration curve, choose this option only if the calibration mode defined in the method is curve) or an ‘unknown’. For standard chromatograms, it is compulsory to complete the ‘level’ and the ‘calibration’ fields.

Start the sequence by clicking the button.
To view the current acquisition, select the “system” tab and then the system name.
After each acquisition, a chromatogram is generated and available for processing (FILE / OPEN / OPEN CHROMATOGRAM). If standards have been defined the calibration curve is generated, display it in the ‘calibration’ tab, by using the FILE / OPEN / OPEN CALIBRATION CURVE menu.

How to Build a Process Method

(Integration, identification, quantification and printing)

It is recommended that the process sections of the method to be done after the acquisition of a chromatogram, typical of the analysis to be performed. In the first step, the parameters are in the chromatogram method; once completed the method is extracted from the chromatogram and a method file is generated. This method will be used to acquire and to reprocess other chromatograms.

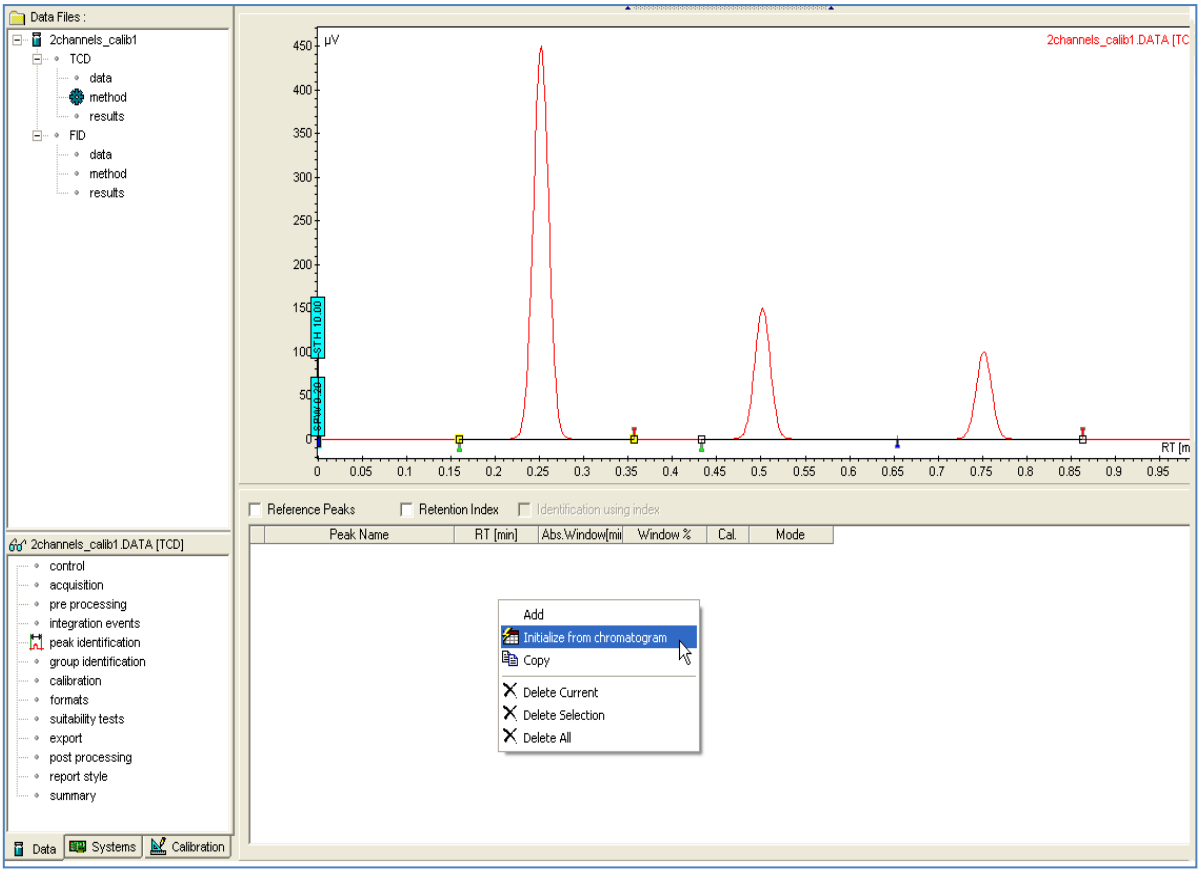
Remember that a method file contains all of the useful information, from acquisition to report printing via integration, identification, quantification etc.

1. Acquire a chromatogram with a minimal method (refer to page 241).

   Open the generated chromatogram, select the method part.
   Complete the following parts:

   - Integration: define the integration events to obtain the optimum integration (See page 43 for the details of each event). Once an event is defined, click on the icon to apply changes. Changes are immediately taken into account and integration results are available for viewing in the chromatogram results part.
   - Peak identification:

   Click on the right mouse button and select the ‘Initialize from chromatogram’ option.



The retention times of all integrated peaks of the chromatogram are displayed. Type a name for the peaks of interest and delete any lines which are not of interest (select the entire line, click on the right mouse button, Delete Current). Define the identification windows and the identification mode (refer to page 65).

- Group identification: refer to page 73.
- Calibration: The user must configure the calibration parameters in this subsection.

Two examples are described:

Example 1: Response in area, external standard, with a calibration curve of 3 levels with averaging, results displayed in µg/L, process unknown peaks with a response factor of 0.59.

- Click on “external standard”,
- Click on the Initialize from peak ID button, to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatic.
- Define the parameters: area response, curve response factor, standard quantities in the identification table (define the column number using the parameter “level number”, check the “average levels” box to, average points of the same level before drawing the curve), enter a curve name (the generated file will contain all the calibration curves generated, by compound), define the unknown peaks process.

The calibration method section is now complete. To use this method, to acquire or reprocess other chromatograms, it must be extracted. For this save it via the menu: FILE / SAVE AS / SAVE METHOD AS. Give a name to the method. The method is created for the system associated with the chromatogram used for its creation.

Example 2: Response in height, internal standard with normalization to 75.8%, subtracting the internal standard(s) quantity (ies) of final results, use response factors entered by user, reprocess the unknown compounds as one of the identified and quantified compound.

Click on “internal standard”

Click on Initialize from peak ID button to import all the identified peaks, or check the Cal. Box of each peak of interest in the identification table to make the import automatic.

The user must define which peak(s) is (are) internal standard(s), by checking the corresponding box in the calibration table.

Set the other parameters: responses in height, manual factors, check the “normalize to” box and enter the normalization percentage, check the ‘subtract ISTD mass’ to subtract the internal standard quantity (ies) from results. In the unknown compounds process, select “reference component” and define in the “Standard” box the name of the associated internal standard.

- The calibration method section is complete. To use this method, to acquire or reprocess other chromatograms, it must be extracted. For this save it via the menu: FILE / SAVE AS / SAVE METHOD AS. Give a name to the method. The method is created for the system associated with the chromatogram used for its creation; the control section must still be completed.

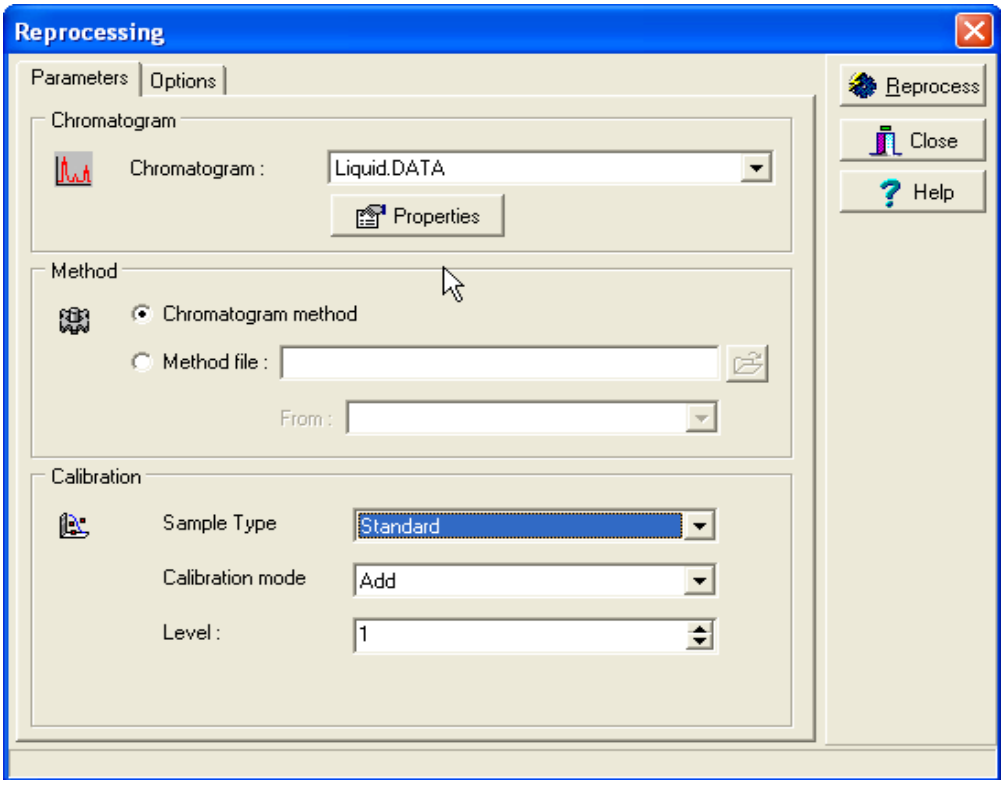
How to Reprocess a Chromatogram

(To integrate, quantify, print a report for a standard or an unknown sample)

There are two ways to reprocess a chromatogram, the reprocessing of an individual chromatogram, or the reprocessing of a series of chromatograms using a reprocessing list.

Individual chromatograms reprocess:

1. Open the chromatogram to reprocess.
2. Menu PROCESSING / REPROCESS, complete the following screen (reference to ‘Single Reprocessing’ section).

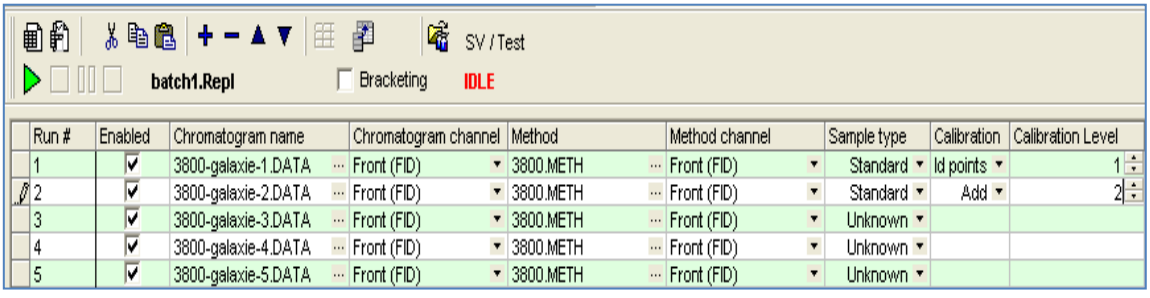


In the method section, choose the chromatogram method or another method selected in the field “method file”. In the calibration part, specify the sample type: an unknown or a standard of level (I). If the chromatogram is a standard (calibration point generation), the user can choose to overwrite an existing curve by checking the “Clear old points” box, to overwrite all the points of the same level already built by checking the “Clear this level only” box or to add the point to an existing curve (do not check anything). If the chromatogram is an unknown, do not check anything.

3. Click on the reprocess button. When the ‘Processing done’ message is displayed, the chromatogram is reprocessed.
4. Click on the Close button. The results are immediately updated in the chromatogram.

Reprocess simultaneously several chromatograms (refer to the Reprocessing Several Acquisitions: The Reprocessing List section, page 176).

Create a reprocessing list. Menu FILE / NEW / NEW REPROCESSING LIST.


SV / Test
batch1.Repl
Bracketing
IDLE
Run # | Enabled | Chromatogram name | Chromatogram channel | Method | Method channel | Sample type | Calibration | Calibration Level
1 | 3800-galaxie-1.DATA | Front (FID) | 3800.METH | Front (FID) | Standard | Id points | 1
2 | 3800-galaxie-2.DATA | Front (FID) | 3800.METH | Front (FID) | Standard | Add | 2
3 | 3800-galaxie-3.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown
4 | 3800-galaxie-4.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown
5 | 3800-galaxie-5.DATA | Front (FID) | 3800.METH | Front (FID) | Unknown

Select in the ‘Chromatogram name’ field, the chromatograms to be reprocessed, specify the method name to be used in the corresponding field, complete the ‘sample type’ field (specifying whether the chromatogram is an unknown or a standard). If the chromatogram is a standard, the ‘Calibration level’ and ‘Calibration’ columns must be completed.

Depending on the parameters defined in the method, fill in the other fields as necessary.

Start the reprocessing list by clicking on .
Once the reprocess is completed, open the chromatograms and view the results or checkthe printed report if any printing was defined in the method.

NOTE: Chromatograms selected in a reprocessing list must be closed in CompassCDS to be reprocessed

How to Build a Calibration Curve

A calibration curve can be created either automatically during the acquisition, or after by reprocessing chromatograms.

Creating a calibration curve during the acquisition: (see page 160)

Create a method; fill in at least the identification and calibration parts, as mentioned in “The different Parts of the Method” section.

Acquire chromatograms, either using a Quick Start or a sequence (see page 139).

In the case of a simple acquisition, complete the ‘Quick Start’ windows in the ‘calibration’ field; define the sample type using the scrolling menu (standard of level 1, standard of level 2, etc.). Check ‘clear old points’ to overwrite an existing calibration curve, ‘clear this level only’ to overwrite all the points of the same level or do not check anything to add the point to the existing calibration curve. Start the acquisition and the corresponding calibration point is created.

In the case of a sequence, specify in the ‘Sample Type’ column which chromatograms are standards by selecting ‘standard’. For all these standards, it is compulsory to associate a corresponding level number in the column ‘Level’ and select the appropriate option in the ‘calibration’ column: ‘clear old points’ to overwrite an existing calibration curve, ‘clear this level only’ to overwrite all the points of the same level or do not check anything to add the point to the existing calibration curve.

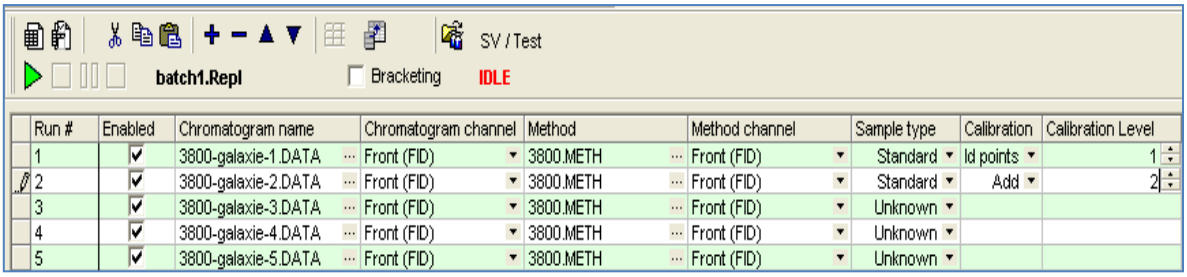
Creating a calibration curve after the chromatogram acquisition (see page 160)

Create a method; fill in at least the identification and calibration parts, as mentioned in ‘The different Parts of the Method’ section.

The process can be made in two ways: using the REPROCESS function to reprocess one chromatogram after the other, or using a Reprocessing list to reprocess several chromatograms.

REPROCESS: The chromatograms to reprocess must be open, select the menu PROCESSING / REPROCESS and follow the instructions defined in the Single Reprocessing section.

Reprocessing list (see page 176)



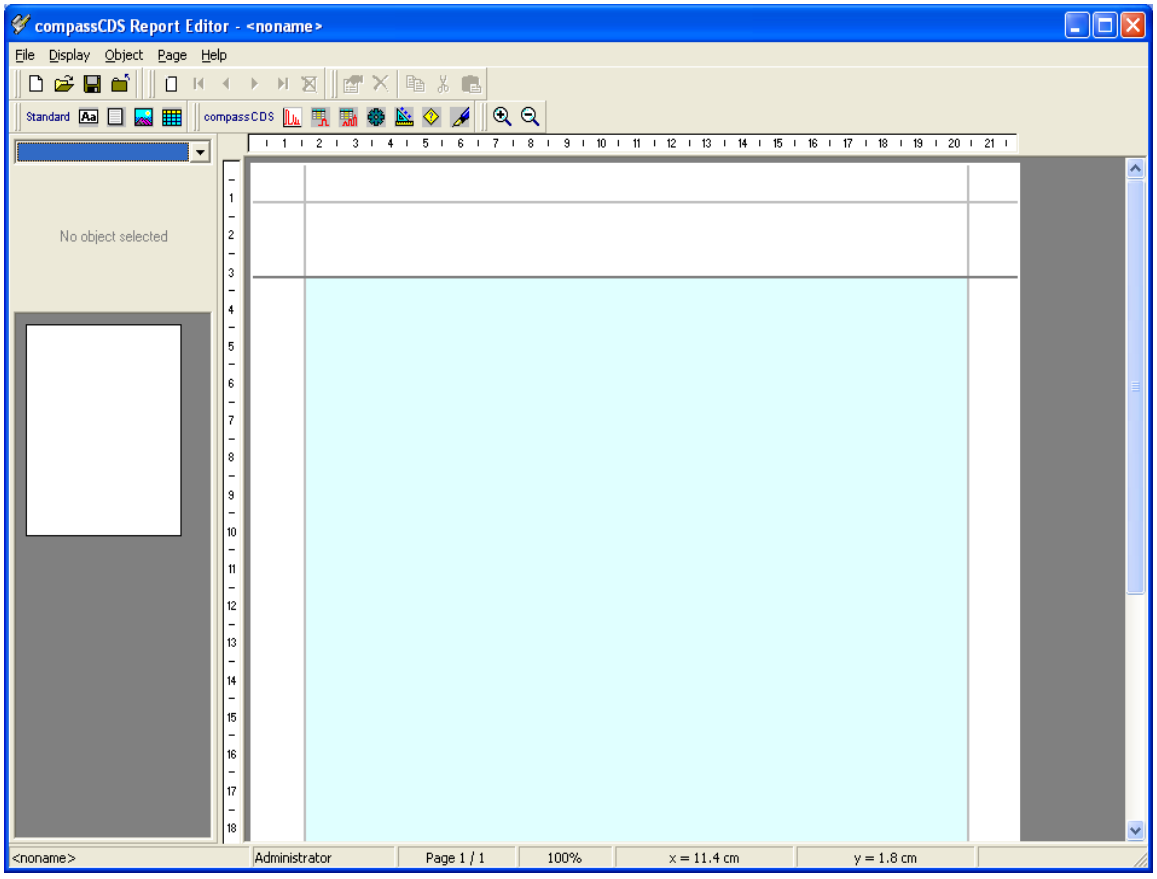
Run #	Enabled	Chromatogram name	Chromatogram channel	Method	Method channel	Sample type	Calibration	Calibration Level
1	☑	3800-galaxie-1.DATA	Front (FID)	3800.METH	Front (FID)	Standard	Id points	1
2	☑	3800-galaxie-2.DATA	Front (FID)	3800.METH	Front (FID)	Standard	Add	2
3	☑	3800-galaxie-3.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		
4	☑	3800-galaxie-4.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		
5	☑	3800-galaxie-5.DATA	Front (FID)	3800.METH	Front (FID)	Unknown		

Select the chromatograms to be reprocessed in the ‘Chromatogram name’ column, specify the name of the method to be used in the corresponding field and complete the ‘sample type’ column. For the standard chromatograms do not forget to fill in both ‘Calibration level’ and ‘Calibration’ columns.

Depending on the parameters defined in the method, fill in the other fields.

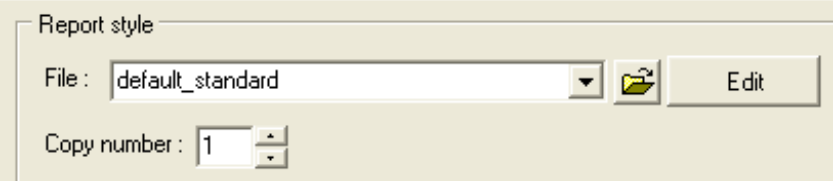
How to Print a Customized Report

1. A report template must first be created, define the objects to be printed: chromatogram, result table, calibration curve, text, etc. This template is created from CompassCDS Report Editor. Select the FILE / NEW / NEW REPORT STYLE menu. The CompassCDS Report Editor interface is displayed:



Define the template (refer to the CompassCDS Report Editor user’s Guide), save it and close the CompassCDS Report Editor.

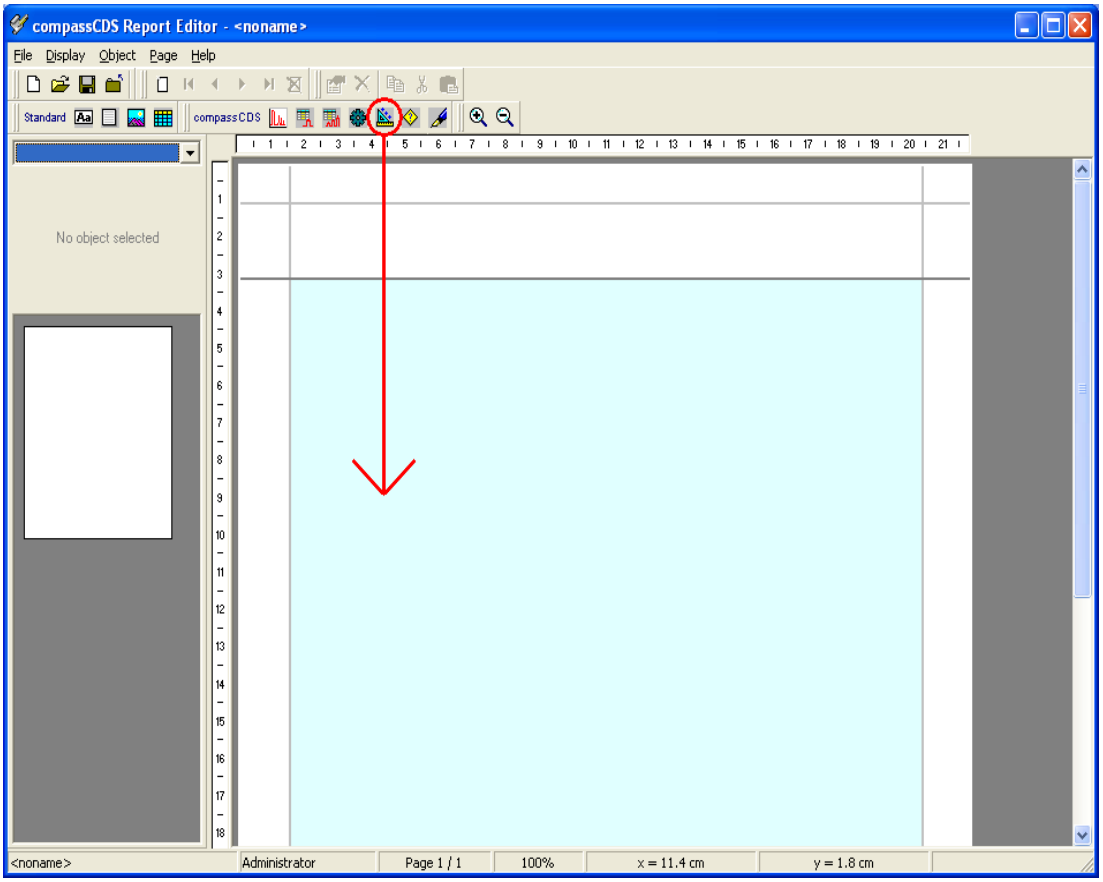
In the CompassCDS Chromatography Data System, in the ‘Report style’ part of the method, select the template name in the ‘File’ box, and define the number of reports to be printed.



Report printing is automatic during an acquisition (QUICK START), a sequence, a reprocessing list or a reprocess using the function, using a method in which a template and at least one printing is specified. Nevertheless, it is possible to do all these functions without printing the report by un-checking the printing option in the “Options” tab of the REPROCESS or of the QUICK START or in the “Method properties” column of the sequence or of the reprocessing list.

How to Print a Calibration Curve

1. Create a calibration curve (see “The Calibration Curves section” page 160).
2. Create a report style in the CompassCDS Report Editor, for which the calibration curve object is specified.



Open a chromatogram whose method contains a calibration curve name (‘Calibration’ section) and then print by clicking on the icon.

Two options are available:

- Printing from a chromatogram: open a chromatogram, define a report style in which the Calibration curve object is defined in the corresponding part of its method, and then click on the icon.
- Printing from a calibration curve by clicking on the icon.

Glossary

External standard: The external standard calibration allows calculation of the identified peak quantities, using a calibration curve or a manual response factor, which is entered by the user.

CompassCDS Configuration Manager: It is CompassCDS maintenance manager. It allows the user to declare, configure, manage chromatographic systems, and define the user base (users, groups, projects, profiles).

CompassCDS Report Editor: It is the report printing manager of CompassCDS.

Internal standard: Internal standard calibration requires the addition of a known quantity of defined compound(s) in every sample to be analyzed. In the same way as for the external standard, a calibration curve is created or manual response factors entered. The calibration curve created takes into account the internal standard quantity associated with the compound. This calculation method is used more in gas chromatography to compensate for the inaccuracy of the injection volume (manual injection).

Method templates: The method templates are models for new methods (not compulsorily defined on the same system). For reusing variables, chromatograms or peak report formats, etc. with other methods, save the current method as a template which you can then use to create a new method. The method template uses the entire method, except the instrument control section.

Popup menu: A popup menu is a menu associated with an object and hidden most of the time. To view the popup menu of an object, position the cursor inside the object and press the right mouse button. Then choose any item of the popup menu with the left mouse button. The object can be a curve, a table, a browser, etc.

Standalone: This term concerns the configuration mode of the software. It means that the software is not set for a network configuration, but is used locally on one computer.

System variables: Many variables allowing for specific calculations on peaks, groups or global chromatogram are available in CompassCDS. These variables are calculated automatically for each chromatogram.

User input variables: As opposed to a system variable, a user input is created by the user. Two user input types exist: the user input for which user must then enter a value or text and the user formula for which the user creates customized calculations, not made by default in CompassCDS.

Workstation: It is the name of the computer on which the software is installed.

See also the CompassCDS Configuration Manager User Guide Glossary.